Electronic Supplementary Information

Indolo-Quinoline Boron Difluoride Dyes：Synthesis and Spectroscopic Properties

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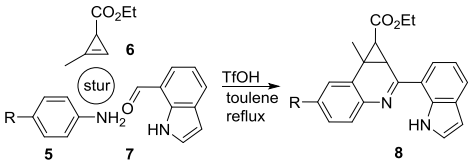
1. General Information

All solvents were purified by standard methods. ^{1}H and ^{13}C NMR spectra were recorded on 400 MHz and 101 MHz spectrometer, respectively. Chemical shifts (in ppm) were calibrated with the solvent residual $CHCl_3$ peak or/and referenced to tetramethylsilane (δ = 0 ppm) in deuterated chloroform. The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad. All reactions were monitored by thin-layer chromatography (TLC) analysis, which was visualized by UV light (254 nm) and acidic ceric ammonium molybdate. HRMS (ESI) data were obtained using a Fourier transform ion cyclotron resonance mass spectrometer. Flash column chromatography was carried out using silica gel (300-400 mesh). All commercially available starting materials were used directly without further purification.

DFT calculations. The ground state structures of dyes **9a**, **9c**, **9f**, **9g**, **9i**, **10**, **11** were optimized using DFT with B3LYP functional and 6-31G(d) basis set. The geometry of the molecules were optimized with Gaussian 09 package[1] at B3LYP/6-31G(d) computational level. The minimum nature of the structure was confirmed by frequency calculations at the same computational level. The excited state related calculations (UV-vis absorption) were carried out with the time dependent DFT (TDDFT) with the optimized structure of the ground state (DFT/6-31+G(d,p)). The excitation of the fluorophores was calculated based on the optimized excited state geometry. All of these calculations were performed with Gaussian 09 (Revision A.02).

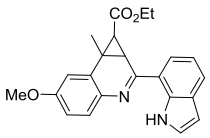
2. Experimental Section

2.1 General procedure for Povarov-type reaction.



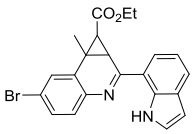
To a solution containing aromatic aldehyde (**7**) (0.22 mmol, 2.2 eq.), cyclopropene (**6**) (0.10 mmol, 1.0 eq.) and aniline (**5**) (0.20 mmol, 2.0 eq.) in 1.0 mL of toluene was added triflic acid (0.005 mmol, 5 mol%), and the resulting mixture was stirred for 5-14 h at 110 °C using Dean-Stark trap. Then the reaction was quenched with saturated aqueous $NaHCO_3$ solution at 0 °C. The organic layer was washed with brine, dried over Na_2SO_4, and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel, eluting with petroleum ether/EtOAc to give product **8**.

Ethyl 2-(1*H*-indol-7-yl)-5-methoxy-7b-methyl-1a,7b-dihydro-1*H*-cyclopropa[*c*]quinoline-1-carboxylate (8a).



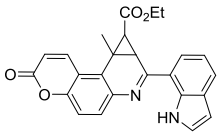
The reaction was performed according to the general procedure, after purification by column chromatography on silica gel (PE/EtOAc = 20/1), affording **8a** (17.0 mg, 45% yield). R_f = 0.53 (PE/EtOAc = 5/1); light yellow solid: ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.43 (s, 1H), 7.80 (dd, *J* = 7.6, 2.8 Hz, 2H), 7.58 (d, *J* = 8.8 Hz, 1H), 7.38 (t, *J* = 2.8 Hz, 1H), 7.23 (t, *J* = 7.6 Hz, 1H), 7.15 (d, *J* = 2.8 Hz, 1H), 6.91 (dd, *J* = 8.8, 2.8 Hz, 1H), 6.61 (t, *J* = 2.8 Hz, 1H), 4.25 (q, *J* = 7.2 Hz, 2H), 3.90 (s, 3H), 3.44 (d, *J* = 5.2 Hz, 1H), 1.80 (s, 3H), 1.41 (d, *J* = 5.2 Hz, 1H), 1.30 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.1, 160.6, 158.9, 135.4, 134.4, 130.7, 130.3, 128.9, 124.8, 124.1, 122.4, 120.4, 119.2, 112.7, 111.4, 102.2, 61.3, 55.6, 31.6, 30.6, 28.2, 16.8, 14.3. HRMS (ESI) m/z: Calcd for $C_{23}H_{23}N_2O_3$ $[M+H]^+$ 375.1709; Found 375.1708. MP: 162–163 °C.

Ethyl 5-bromo-2-(1*H*-indol-7-yl)-7b-methyl-1a,7b-dihydro-1*H*-cyclopropa[*c*]quinoline-1-carboxylate (8b).



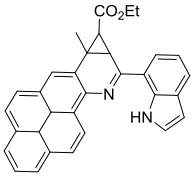
The reaction was performed according to the general procedure, after purification by column chromatography on silica gel (PE/EtOAc = 15/1), affording **8b** (16.0 mg, 38% yield). R_f = 0.49 (PE/EtOAc = 5/1); light yellow solid: ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.35 (s, 1H), 7.84 (dd, *J* = 7.6, 4.8 Hz, 2H), 7.75 (d, *J* = 2.0 Hz, 1H), 7.52 – 7.47 (m, 2H), 7.38 (dd, *J* = 3.2, 2.4 Hz, 1H), 7.23 (d, *J* = 7.6 Hz, 1H), 6.63 (dd, *J* = 3.2, 2.4 Hz, 1H), 4.26 (q, *J* = 7.2 Hz, 2H), 3.49 (d, *J* = 5.2 Hz, 1H), 1.79 (s, 3H), 1.39 (d, *J* = 5.2 Hz, 1H), 1.31 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.5, 163.8, 140.4, 134.5, 131.1, 130.7, 130.4, 129.0, 128.9, 125.02, 124.96, 123.1, 120.5, 120.0, 119.3, 102.3, 61.5, 31.1, 30.6, 28.2, 16.8, 14.3. HRMS (ESI) m/z: Calcd for $C_{22}H_{20}N_2O_2Br$ $[M+H]^+$ 423.0708; Found 423.0704. MP: 151–153 °C.

Ethyl 2-(1*H*-indol-7-yl)-9c-methyl-7-oxo-1,1a,7,9c-tetrahydrocyclopropa[*c*]pyrano[3,2-f]quinoline-1-carboxylate (8c).



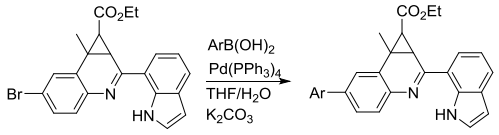
The reaction was performed according to the general procedure, after purification by column chromatography on silica gel (PE/EtOAc = 5/1), affording **8c** (13.0 mg, 32% yield). R_f = 0.15 (PE/EtOAc = 5/1); yellow solid: ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.29 (s, 1H), 8.24 (d, *J* = 10.0 Hz, 1H), 7.86 (d, *J* = 8.0 Hz, 1H), 7.80 (d, *J* = 8.8 Hz, 2H), 7.40 (t, *J* = 2.8 Hz, 1H), 7.35 (d, *J* = 8.8 Hz, 1H), 7.26 (t, *J* = 8.0 Hz, 1H), 6.72 – 6.61 (m, 1H), 6.52 (d, *J* = 9.6 Hz, 1H), 4.51 – 4.23 (m, 2H), 3.24 (d, *J* = 5.6 Hz, 1H), 1.89 (s, 1H), 1.68 (d, *J* = 5.6 Hz, 3H), 1.36 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.2, 163.2, 159.9, 154.0, 141.0, 138.4, 134.4, 133.0, 129.1, 126.6, 125.3, 125.1, 123.3, 119.8, 119.4, 117.4, 117.0, 116.1, 102.5, 61.8, 31.4, 27.5, 24.7, 22.9, 14.4. HRMS (ESI) m/z: Calcd for $C_{25}H_{21}N_2O_4$ $[M+H]^+$ 413.1501; Found 413.1504. MP: 235–237 °C.

Ethyl 8-(1*H*-indol-7-yl)-6b-methyl-3a^1,5a^1,6b,7a-tetrahydro-7*H*-cyclopropa[*c*]phenaleno[1,9-*gh*]quinoline-7-carboxylate (8d).



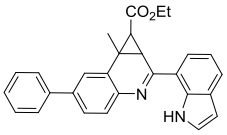
The reaction was performed according to the general procedure, after purification by column chromatography on silica gel (PE/EtOAc = 15/1), affording **8d** (9.0 mg, 19% yield). R_f = 0.50 (PE/EtOAc = 5/1); yellow green solid: ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.44 (s, 1H), 9.05 (d, *J* = 9.2 Hz, 1H), 8.44 (s, 1H), 8.29 (d, *J* = 9.2 Hz, 1H), 8.24 (d, *J* = 7.6 Hz, 1H), 8.21 (d, *J* = 7.6 Hz, 1H), 8.09 (s, 2H), 8.03 (t, *J* = 7.6 Hz, 1H), 7.96 (d, *J* = 7.6 Hz, 1H), 7.90 (d, *J* = 7.6 Hz, 1H), 7.54 (dd, *J* = 2.8, 2.0 Hz, 1H), 7.32 (t, *J* = 7.6 Hz, 1H), 6.72 (t, *J* = 6.4 Hz, 1H), 4.30 (q, *J* = 7.2 Hz, 2H), 3.75 (d, *J* = 5.2 Hz, 1H), 2.11 (s, 3H), 1.49 (d, *J* = 5.2 Hz, 1H), 1.31 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.2, 162.4, 135.1, 134.3, 131.3, 131.0, 130.1, 129.0, 128.4, 128.2, 127.8, 127.1, 127.0, 126.2, 125.6, 125.4, 125.0, 124.8, 124.7, 124.5, 123.5, 122.9, 122.2, 121.3, 119.6, 102.5, 61.4, 32.6, 32.3, 29.2, 17.7, 14.3. HRMS (ESI) m/z: Calcd for $C_{32}H_{27}N_2O_2$ $[M+H]^+$ 471.2067; Found 471.2068.

2.2 General procedure for Suzuki reaction.



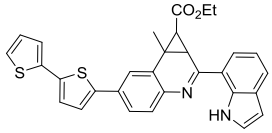
A mixture of **8b** (0.10 mmol), aromatic boronic acid (0.12 mmol) and $Pd(PPh_3)_4$ (0.0010 mmol) in THF (2.0 mL), and aqueous K_2CO_3 (1 N, 1.0 mL) was refluxed for 5 h under an argon atmosphere. After the **8b** had been completely consumed, as indicated by TLC, the organic layer was washed with brine, dried over Na_2SO_4, and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel, eluting with petroleum ether/EtOAc to give product **8e−8h**.

Ethyl 2-(1*H*-indol-7-yl)-7b-methyl-5-phenyl-1a,7b-dihydro-1*H*-cyclopropa[*c*]quinoline-1-carboxylate (8e).



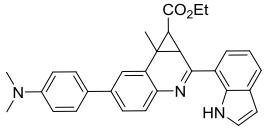
The reaction was performed according to the general procedure, after purification by column chromatography on silica gel (PE/EtOAc = 15/1), affording **8e** (40.0 mg, 95% yield). R_f = 0.52 (PE/EtOAc = 5/1); light yellow solid: ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.48 (s, 1H), 7.86 – 7.83 (m, 3H), 7.72 – 7.67 (m, 3H), 7.60 (dd, *J* = 8.0, 2.0 Hz, 1H), 7.48 (t, *J* = 7.6 Hz, 2H), 7.40 – 7.36 (m, 2H), 7.25 (t, *J* = 7.6 Hz, 1H), 6.63 (dd, *J* = 3.2, 2.4 Hz, 1H), 4.26 (q, *J* = 7.2 Hz, 2H), 3.52 (d, *J* = 5.2 Hz, 1H), 1.87 (s, 3H), 1.46 (d, *J* = 5.2 Hz, 1H), 1.30 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.9, 163.3, 140.7, 140.6, 140.2, 134.5, 129.6, 129.5, 129.0, 128.9, 127.5, 127.1, 126.3, 124.9, 124.7, 124.5, 123.0, 120.3, 119.3, 102.3, 61.4, 31.6, 30.9, 28.5, 17.0, 14.3. HRMS (ESI) m/z: Calcd for $C_{28}H_{25}N_2O_2$ $[M+H]^+$ 421.1916; Found 421.1916. MP: 178–179 °C.

Ethyl 6-[(2,2'-bithiophen)-5-yl]-2-(1*H*-indol-7-yl)-7b-methyl-1a,7b-dihydro-1*H*-cyclopropa[*c*]quinoline-1-carboxylate (8f).



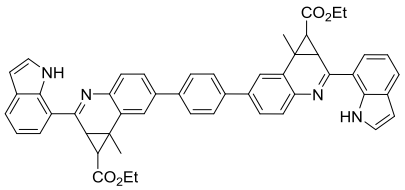
The reaction was performed according to the general procedure, after purification by column chromatography on silica gel (PE/EtOAc = 15/1), affording **8f** (45.0 mg, 89% yield). R_f = 0.50 (PE/EtOAc = 5/1); yellow green solid: ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.44 (s, 1H), 7.89 – 7.81 (m, 3H), 7.63 (t, *J* = 8.0 Hz, 1H), 7.60 (dd, *J* = 8.0, 2.0 Hz, 1H), 7.40 (dd, *J* = 2.8, 2.4 Hz, 1H), 7.31 (d, *J* = 3.6 Hz, 1H), 7.27 – 7.23 (m, 3H), 7.19 (d, *J* = 3.6 Hz, 1H), 7.05 (dd, *J* = 5.2, 3.6 Hz, 1H), 6.63 (dd, *J* = 3.2, 2.4 Hz, 1H), 4.27 (q, *J* = 7.2 Hz, 2H), 3.51 (d, *J* = 4.8 Hz, 1H), 1.88 (s, 3H), 1.47 (d, *J* = 5.2 Hz, 1H), 1.31 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.8, 163.2, 142.5, 140.9, 137.3, 137.1, 134.5, 133.0, 129.9, 129.6, 129.0, 127.9, 125.0, 124.8, 124.72, 124.68, 124.5, 124.1, 123.7, 123.0, 122.9, 120.2, 119.3, 102.3, 61.4, 31.5, 30.9, 28.5, 16.9, 14.3. HRMS (ESI) m/z: Calcd for $C_{30}H_{25}N_2O_2S$ $[M+H]^+$ 509.1357; Found 509.1354. MP: 95–97 °C.

Ethyl 5-[4-(dimethylamino)phenyl]-2-(1*H*-indol-7-yl)-7b-methyl-1a,7b-dihydro-1*H*-cyclopropa[*c*]quinoline-1-carboxylate (8g).



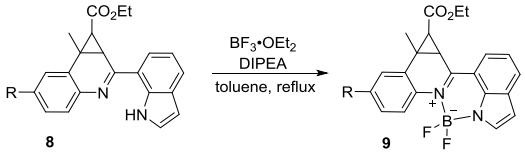
The reaction was performed according to the general procedure, after purification by column chromatography on silica gel (PE/EtOAc = 15/1), affording **8g** (42.0 mg, 91% yield). R_f = 0.41 (PE/EtOAc = 5/1); yellow solid: ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.50 (s, 1H), 7.85 – 7.80 (m, 3H), 7.66 (d, *J* = 8.0 Hz, 1H), 7.61 – 7.58 (m, 2H), 7.56 (dd, *J* = 8.0, 2.0 Hz, 1H), 7.40 (t, *J* = 2.8 Hz, 1H), 7.24 (t, *J* = 7.6 Hz, 1H), 6.84 (d, *J* = 8.8 Hz, 2H), 6.63 (t, *J* = 2.8 Hz, 1H), 4.26 (q, *J* = 7.2 Hz, 2H), 3.49 (d, *J* = 5.2 Hz, 1H), 3.03 (s, 6H), 1.87 (s, 3H), 1.46 (d, *J* = 5.2 Hz, 1H), 1.30 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.1, 162.4, 150.2, 140.4, 139.7, 134.6, 129.5, 129.4, 129.0, 128.5, 127.7, 125.3, 124.9, 124.4, 123.4, 122.7, 120.5, 119.3, 112.8, 102.2, 61.3, 40.5, 31.7, 30.9, 28.5, 17.0, 14.3. HRMS (ESI) m/z: Calcd for $C_{30}H_{30}N_3O_2$ $[M+H]^+$ 464.2338; Found 464.2337. MP: 195–197 °C.

Ethyl 5-{4-[2-(1*H*-indol-7-yl)-7b-methyl-1-(propionyloxy)-1a,7b-dihydro-1*H*-cyclopropa[*c*]quinolin-5-yl] phenyl}-2-(1*H*-indol-7-yl)-7b-methyl-1a,7b-dihydro-1*H*-cyclopropa[*c*]quinoline-1- carboxylate (8h).



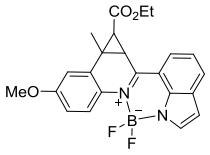
The reaction was performed at 0.05 mmol scale according to the general procedure, after purification by column chromatography on silica gel (PE /EtOAc = 10/1), affording **8h** (32.0 mg, 84% yield). R_f = 0.43 (PE/EtOAc = 5/1); light yellow solid: ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.50 (s, 2H), 7.92 (d, *J* = 2.0 Hz, 2H), 7.87 (t, *J* = 7.6 Hz, 4H), 7.80 (s, 4H), 7.75 (d, *J* = 8.0 Hz, 2H), 7.68 (dd, *J* = 8.0, 2.0 Hz, 2H), 7.42 (t, *J* = 2.8 Hz, 2H), 7.27 (dd, *J* = 9.6, 6.0 Hz, 2H), 6.65 (t, *J* = 2.8 Hz, 2H), 4.29 (q, *J* = 7.2 Hz, 4H), 3.55 (d, *J* = 5.3 Hz, 2H), 1.92 (s, 6H), 1.50 (d, *J* = 5.2 Hz, 2H), 1.32 (t, *J* = 7.2 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.9, 163.4, 140.8, 139.7, 139.5, 134.5, 129.7, 129.6, 129.0, 127.5, 126.2, 125.0, 124.8, 124.4, 123.0, 120.3, 119.3, 102.3, 61.4, 31.6, 30.9, 28.5, 17.0, 14.3. HRMS (ESI) m/z: Calcd for $C_{50}H_{43}N_4O_4$[M+H]$^+$ 763.3284; Found 763.3296. MP: 178–180 °C.

2.3 General procedure for synthesis of BF_2 complexes.



Ligand **8** (0.05 mmol) was dissolved in dry toluene (1 mL). *N,N*-Diisopropylethylamine (0.15 mmol) and boron trifluoride diethyl ether complex (0.15 mmol) were added to the solution and the mixture was refluxed for 6 h. Then water was added to the solution. The solution was extracted with CH_2Cl_2. The organic layer was dried over Na_2SO_4. After concentration of solvent, the residue was purified via chromatography on silica gel to give product **9**.

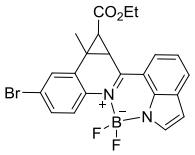
Compound 9a (BF_2@8a−H).



The reaction was performed according to the general procedure, after purification by column chromatography on silica gel (PE/EtOAc = 15/1), affording **9a** (20.0 mg, 95% yield). R_f = 0.43 (PE/EtOAc = 10/1); yellow green solid: ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.62 (dd, *J* = 9.6, 4.2 Hz, 1H), 8.00 (d, *J* = 7.8 Hz, 1H), 7.91 (d, *J* = 7.8 Hz, 1H), 7.64 (d, *J* = 3.0 Hz, 1H), 7.25 (t, *J* = 7.8 Hz, 3H), 7.15 (d, *J* = 3.0 Hz, 1H), 6.95 (dd, *J* = 9.6, 3.0 Hz, 1H), 6.72 (d, *J* = 3.0 Hz, 1H), 4.27 (q, *J* = 7.2 Hz, 2H), 3.91 (s, 3H), 3.87 (d, *J* = 4.8 Hz, 1H), 1.86 (s, 3H), 1.76 (d, *J* = 5.4 Hz, 1H), 1.30 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 169.9, 163.0, 159.4, 135.5, 132.2, 129.8, 129.6,

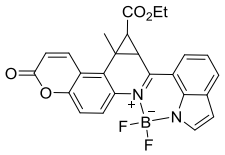
129.0, 127.9 (t, *J* = 10.5 Hz), 127.7, 122.9, 119.8, 112.7, 111.9, 104.4, 62.0, 55.6, 31.7, 30.3, 29.8, 16.7, 14.2. HRMS (ESI) m/z: Calcd for $C_{23}H_{22}BN_2O_3F_2[M+H]^+$ 423.1692; Found 423.1685.

Compound 9b (BF_2@8b−H).



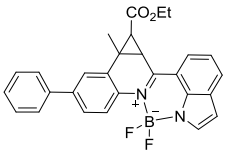
The reaction was performed according to the general procedure, after purification by column chromatography on silica gel (PE/EtOAc = 10/1), affording **9b** (23.0 mg, 98% yield). R_f = 0.40 (PE/EtOAc = 5/1); yellow green solid: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.53 (dd, *J* = 9.2, 4.0 Hz, 1H), 8.04 (d, *J* = 7.6 Hz, 1H), 7.94 (d, *J* = 8.0 Hz, 1H), 7.77 (d, *J* = 2.0 Hz, 1H), 7.63 (d, *J* = 3.2 Hz, 1H), 7.54 (dd, *J* = 9.2, 2.4 Hz, 1H), 7.26 (t, *J* = 8.0 Hz, 1H), 6.73 (d, *J* = 3.2 Hz, 1H), 4.28 (q, *J* = 7.2 Hz, 2H), 3.90 (d, *J* = 4.8 Hz, 1H), 1.86 (s, 3H), 1.75 (d, *J* = 4.8 Hz, 1H), 1.31 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.3, 165.6, 135.8, 133.2, 132.2, 131.2, 130.7, 130.0, 129.3, 129.1, 127.7 (t, *J* = 7.0 Hz), 123.7, 122.5, 120.1, 112.4, 104.7, 62.2, 31.2, 30.7, 29.8, 16.7, 14.2. HRMS (ESI) m/z: Calcd for $C_{22}H_{19}BN_2O_2F_2Br$ $[M+H]^+$ 471.0689; Found 471.0659.

Compound 9c (BF_2@8c−H).



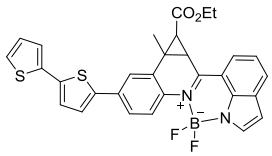
The reaction was performed according to the general procedure, after purification by column chromatography on silica gel (PE/EtOAc = 1/1), affording **9c** (21.0 mg, 91% yield). R_f = 0.30 (PE/EtOAc = 1/1); light yellow solid: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.85 (d, *J* = 9.2 Hz, 1H), 8.13 (d, *J* = 10.0 Hz, 1H), 8.06 (d, *J* = 7.6 Hz, 1H), 7.91 (d, *J* = 8.0 Hz, 1H), 7.65 (d, *J* = 2.8 Hz, 1H), 7.40 (d, *J* = 9.6 Hz, 1H), 7.29 (t, *J* = 7.7 Hz, 1H), 6.75 (d, *J* = 3.2 Hz, 1H), 6.57 (d, *J* = 10.0 Hz, 1H), 4.44 – 4.34 (m, 2H), 3.67 (d, *J* = 5.2 Hz, 1H), 2.10 (d, *J* = 5.2 Hz, 1H), 1.90 (s, 3H), 1.39 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.0, 165.0, 159.2, 154.1, 140.0, 135.9, 131.3, 131.2, 130.2, 129.6 (t, *J* = 13.5 Hz), 129.3, 128.3, 124.0, 120.2, 117.5, 117.2, 116.9, 112.5, 104.9, 62.6, 29.8, 26.9, 26.5, 22.3, 14.3. HRMS (ESI) m/z: Calcd for $C_{25}H_{20}BN_2O_4F_2$ $[M+H]^+$ 461.1484; Found 461.1479.

Compound 9e (BF_2@8e−H).



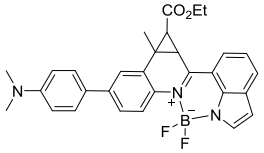
The reaction was performed according to the general procedure, after purification by column chromatography on silica gel (PE/EtOAc = 10/1), affording **9e** (23.0 mg, 98% yield). R_f = 0.42 (PE/EtOAc = 5/1); yellow solid: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.75 (dd, *J* = 8.8, 4.0 Hz, 1H), 8.03 (d, *J* = 7.6 Hz, 1H), 7.96 (d, *J* = 8.0 Hz, 1H), 7.86 (d, *J* = 2.4 Hz, 1H), 7.69 – 7.65 (m, 4H), 7.52 – 7.48 (m, 2H), 7.44 – 7.40 (m, 1H), 7.28 (t, *J* = 7.6 Hz, 1H), 6.75 (d, *J* = 2.8 Hz, 1H), 4.29 (q, *J* = 7.2 Hz, 2H), 3.94 (d, *J* = 4.8 Hz, 1H), 1.95 (s, 3H), 1.82 (d, *J* = 4.8 Hz, 1H), 1.31 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.7, 165.1, 141.3, 139.4, 135.7, 133.3, 130.6, 130.3, 130.0, 129.2, 129.0, 128.2, 127.1, 126.7, 126.5 (t, *J* = 12.0 Hz), 124.6, 123.46, 119.96, 112.6, 104.6, 62.1, 31.8, 30.8, 30.0, 16.9, 14.2. HRMS (ESI) m/z: Calcd for $C_{28}H_{24}BN_2O_2F_2S$ $[M+H]^+$ 469.1899; Found 469.1913.

Compound 9f (BF_2@8f−H).



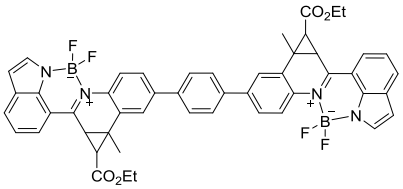
The reaction was performed according to the general procedure, after purification by column chromatography on silica gel (PE/EtOAc = 15/1), affording **9f** (26.0 mg, 94% yield). R_f = 0.41 (PE/EtOAc = 5/1); orange solid: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.66 (dd, *J* = 8.8, 4.0 Hz, 1H), 8.01 (d, *J* = 7.6 Hz, 1H), 7.93 (d, *J* = 7.6 Hz, 1H), 7.80 (d, *J* = 2.0 Hz, 1H), 7.65 (d, *J* = 3.2 Hz, 1H), 7.62 (dd, *J* = 8.8, 2.4 Hz, 1H), 7.33 (d, *J* = 4.0 Hz, 1H), 7.27 – 7.23 (m, 3H), 7.17 (d, *J* = 3.6 Hz, 1H), 7.04 (dd, *J* = 4.8, 3.6 Hz, 1H), 6.73 (d, *J* = 3.2 Hz, 1H), 4.28 (q, *J* = 7.2 Hz, 2H), 3.90 (d, *J* = 4.8 Hz, 1H), 1.93 (s, 3H), 1.80 (d, *J* = 4.8 Hz, 1H), 1.31 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.7, 164.7, 141.0, 138.1, 137.0, 135.7, 134.2, 133.2, 130.9, 130.3, 129.9, 129.2, 128.0, 126.7 (t, *J* = 12.0 Hz), 125.1, 124.84, 124.78, 124.0, 123.4, 122.7, 120.0, 112.6, 104.6, 62.1, 31.6, 30.8, 29.9, 16.8, 14.2. HRMS (ESI) m/z: Calcd for $C_{30}H_{24}BN_2O_2F_2S_2$ $[M+H]^+$ 557.1340; Found 557.1311.

Compound 9g (BF_2@8g−H).



The reaction was performed according to the general procedure, after purification by column chromatography on silica gel (PE/EtOAc = 15/1), affording **9g** (23.0 mg, 90% yield). R_f = 0.35 (PE/EtOAc = 5/1); orange red solid: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.68 (dd, *J* = 8.8, 4.0 Hz, 1H), 8.01 (d, *J* = 7.6 Hz, 1H), 7.94 (d, *J* = 7.6 Hz, 1H), 7.81 (d, *J* = 1.2 Hz, 1H), 7.67 – 7.59 (m, 4H), 7.27 (t, *J* = 8.0 Hz, 1H), 6.83 (d, *J* = 8.8 Hz, 2H), 6.73 (d, *J* = 2.8 Hz, 1H), 4.28 (q, *J* = 7.2 Hz, 2H), 3.91 (d, *J* = 4.8 Hz, 1H), 3.03 (s, 6H), 1.94 (s, 3H), 1.81 (d, *J* = 4.8 Hz, 1H), 1.31 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.0, 164.1, 150.5, 141.4, 135.6, 132.1, 130.5, 129.91, 129.85, 129.1, 127.7, 126.9, 126.4 (t, *J* = 10.7 Hz), 125.5, 123.22, 123.16, 119.8, 112.8, 112.6, 104.4, 62.0, 40.4, 31.9, 30.6, 30.0, 16.9, 14.2. HRMS (ESI) m/z: Calcd for $C_{30}H_{29}BN_3O_2F_2$ $[M+H]^+$ 512.2321; Found 512.2321.

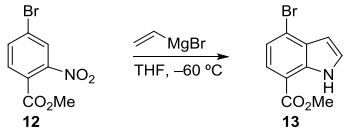
Compound 9h (BF_2@8h−H).



The reaction was performed at 0.025 mmol scale according to the general procedure, after purification by column chromatography on silica gel (PE/EtOAc = 1/1), affording **9h** (20.0 mg, 93% yield). R_f = 0.21 (PE/EtOAc = 1/1); yellow green solid: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.78 (dd, *J* = 8.4, 4.0 Hz, 2H), 8.05 (d, *J* = 7.6 Hz, 2H), 7.98 (d, *J* = 7.6 Hz, 2H), 7.92 (d, *J* = 2.0 Hz, 2H), 7.81 (s, 4H), 7.73 (dd, *J* = 8.8, 2.0 Hz, 2H), 7.68 (d, *J* = 3.2 Hz, 2H), 7.29 (t, *J* = 7.6 Hz, 2H), 6.76 (d, *J* = 2.8 Hz, 2H), 4.30 (q, *J* = 7.2 Hz, 4H), 3.96 (d, *J* = 4.8 Hz, 2H), 1.98 (s, 6H), 1.84 (d, *J* = 4.8 Hz, 2H), 1.32 (t, *J* = 7.2 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.7, 165.2, 140.5, 139.2, 135.8, 133.6, 130.9, 130.8, 130.4, 130.0, 129.2, 127.7, 126.6, 124.4, 123.5, 120.0, 112.6, 104.6, 62.1, 31.8, 30.8, 30.0, 16.9, 14.3. HRMS (ESI) m/z: Calcd for $C_{50}H_{41}B_2N_4O_4F_4$ $[M+H]^+$ 859.3245; Found 859.3249.

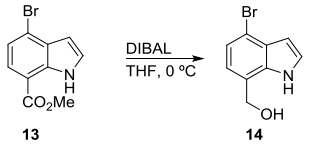
2.4 The procedure for the preparation of 9i.

Methyl 4-bromo-1*H*-indole-7-carboxylate (13).



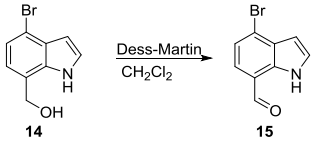
The compound **12** (4.92 g, 19 mmol, 1.0 eq.) was dissolved in dry THF (20 mL) and the solution was cooled to −60 °C under an argon atmosphere. Then, a solution of bromoethenyl-magnesium in THF (20.0 mL) was added dropwise over 30 min. The resulting mixture was allowed to warm to r.t. and stirred for 12 h. Then the reaction was quenched with saturated aqueous $NaHCO_3$ solution at 0 °C. The reaction mixture was extracted with EtOAc. The organic layer was washed with water and brine, dried over Na_2SO_4, and concentrated under vacuum. The residue was purified by column chromatography on silica gel to give **13** as white solid (1.44 g, 30% yield). R_f = 0.42 (PE/EtOAc = 5/1): ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.96 (br, 1H), 7.73 (d, *J* = 8.0 Hz, 1H), 7.37 (t, *J* = 2.8 Hz, 1H), 7.33 (d, *J* = 8.0 Hz, 1H), 6.65 (t, *J* = 2.8 Hz, 1H), 3.98 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.5, 135.7, 129.8, 125.8, 125.0, 122.3, 121.2, 111.9, 103.1, 52.0. HRMS (ESI) m/z: Calcd for $C_{10}H_7BrNO_2$ $[M-H]^-$ 251.9660; Found 251.9658. MP: 139–140 °C.

(4-Bromo-1H-indol-7-yl)methanol (14).



The compound **13** (1.39 g, 5.50 mmol, 1.0 eq.) was dissolved in dry THF (10.0 mL) and the solution was cooled to 0 °C under an argon atmosphere. Then, a solution of DIBAL (14.0 mmol, 2.5 eq.) in THF (10.0 mL) was added dropwise over 30 min. The reaction mixture was stirred for about 4 h at r.t. Then the reaction was quenched with saturated aqueous $NaHCO_3$ solution at 0 °C. After removal of the solvent, the residue was dissolved in ethyl acetate and washed with brine, dried over Na_2SO_4. The dried solution was filtered and the filtrate was concentrated. The residue was purified by column chromatography on silica gel eluting with petroleum ether/EtOAc (2:1) to give **14** as white solid (1.03 g, 83% yield). R_f = 0.33 (PE/EtOAc = 2/1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.08 (br, 1H), 7.27 (t, *J* = 2.8 Hz, 1H), 7.22 (d, *J* = 7.6 Hz, 1H), 6.85 (d, *J* = 7.6 Hz, 1H), 6.61 (t, *J* = 2.8 Hz, 1H), 4.97 (s, 2H), 2.00 (br, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 134.8, 129.1, 124.8, 122.5, 122.2, 120.8, 114.4, 102.9, 64.1. HRMS (ESI) m/z: Calcd for C_9H_7BrNO $[M-H]^-$ 223.9711; Found 223.9713. MP: 88–89 °C.

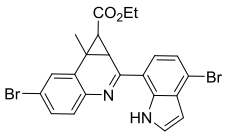
4-Bromo-1H-indole-7-carbaldehyde (15).



To a solution of compound **14** (1.50 g, 6.67 mmol, 1.0 eq) in dichloromethane (15.0 mL), Dess-Martin-Periodinane (DMP) (7.10 g, 16.7 mmol, 2.5 eq) was added at 0 °C. After 10 min the reaction mixture was allowed to warm to room temperature. After completion of the reaction, the mixture was poured into saturated aqueous $NaHCO_3$ solution (15 mL) and stirred well for at least 10 min. After filtration from precipitated benzoic acid the layers were separated, and the aqueous layer was extracted three times with 15 mL of ether. The organic layer was washed with water and brine, dried over Na_2SO_4, and concentrated under vacuum. The residue was purified by column chromatography on silica gel to give **15** as white solid (1.35 g, 91% yield). R_f = 0.45 (PE/EtOAc = 5/1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.25 (br, 1H), 10.09 (s, 1H), 7.50 (d, *J* = 7.6 Hz, 1H), 7.45 (d, *J* = 7.6 Hz, 1H), 7.40 (t, *J* = 2.8 Hz, 1H), 6.68 (t, *J* = 2.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.8, 133.5, 130.1, 129.2, 126.5, 123.4, 122.8, 119.6, 103.2. HRMS (ESI) m/z: Calcd for C_9H_7BrNO $[M-H]^-$ 221.9555; Found

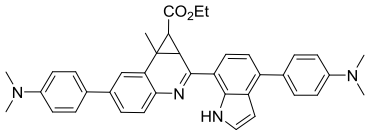
221.9558. MP: 129–131 °C.

Ethyl 6-bromo-2-(4-(4-bromophenyl)-1*H*-indol-7-yl)-7b-methyl-1a,7b-dihydro-1*H*-cyclopropa[*c*]quinoline-1-carboxylate (8j).



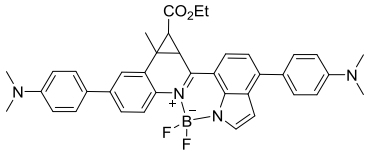
The reaction was performed according to the general procedure (section 2.1), after purification by column chromatography on silica gel (PE/EtOAc = 25/1), affording **8j** (21.0 mg, 45% yield). R_f = 0.56 (PE/EtOAc = 5/1); light yellow solid: ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.47 (s, 1H), 7.74 (t, *J* = 1.2 Hz, 1H), 7.65 (d, *J* = 8.0 Hz, 1H), 7.49 –7.48 (d, *J* = 1.0 Hz, 2H), 7.41 (t, *J* = 3.2 Hz, 1H), 7.39 (d, *J* = 8.0 Hz, 1H), 6.67 (t, *J* = 3.2 Hz, 1H), 4.26 (q, *J* = 7.2 Hz, 2H), 3.41 (d, *J* = 5.2 Hz, 1H), 1.78 (s, 3H), 1.38 (d, *J* = 5.2 Hz, 1H), 1.31 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.3, 163.2, 140.2, 134.5, 131.1, 130.8, 130.5, 129.7, 128.9, 125.6, 123.8, 122.4, 120.8, 119.6, 119.3, 102.8, 61.6, 31.1, 30.5, 28.1, 16.8, 14.3. HRMS (ESI) m/z: Calcd for $C_{22}H_{19}N_2O_2Br_2$ $[M+H]^+$ 500.9813; Found 500.9810. MP: 186–187 °C.

Ethyl 6-[4-(dimethylamino)phenyl]-2-[4-(4-(dimethylamino)phenyl)-1*H*-indol-7-yl]-7b-methyl-1a,7b-dihydro-1*H*-cyclopropa[*c*]quinoline-1-carboxylate (8i).



The reaction was performed at 0.050 mmol scale according to the general procedure (section 2.2), after purification by column chromatography on silica gel (PE/EtOAc = 6/1), affording **8i** (26.0 mg, 89% yield). R_f = 0.22 (PE /EtOAc = 5/1); orange solid: ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.75 (s, 1H), 7.90 (d, *J* = 7.6 Hz, 1H), 7.82 (d, *J* = 1.6 Hz, 1H), 7.72 (d, *J* = 1.6 Hz, 2H), 7.68 (d, *J* = 8.0 Hz, 1H), 7.61 (d, *J* = 8.8 Hz, 2H), 7.57 (dd, *J* = 8.0, 2.0 Hz, 1H), 7.43 (t, *J* = 2.4 Hz, 1H), 7.30 (d, *J* = 7.6 Hz, 1H), 6.91 – 6.84 (m, 5H), 4.28 (q, *J* = 7.2 Hz, 2H), 3.53 (d, *J* = 5.2 Hz, 1H), 3.06 (s, 6H), 3.03 (s, 6H), 1.89 (s, 3H), 1.49 (d, *J* = 4.8 Hz, 1H), 1.31 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.2, 162.1, 150.1, 150.0, 140.01, 139.9, 138.4, 135.1, 129.7, 129.4, 129.3, 128.8, 128.5, 127.7, 126.7, 125.3, 124.7, 123.4, 118.6, 118.4, 112.7, 112.5, 102.1, 61.2, 40.5, 31.7, 30.9, 28.6, 17.0, 14.3. HRMS (ESI) m/z: Calcd for $C_{38}H_{39}N_4O_2$ $[M+H]^+$ 583.3073; Found 583.3070. MP: 234–235 °C.

Compound 9i (BF_2@8i−H).



The reaction was performed according to the general procedure (section 2.3), after purification by column chromatography on silica gel (PE/EtOAc = 5/1), affording **9i** (27.0 mg, 86% yield). R_f = 0.18 (PE/EtOAc = 5/1); red solid: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.65 (dd, *J* = 8.8, 4.0 Hz, 1H), 7.96 (d, *J* = 8.4 Hz, 1H), 7.80 – 7.78 (m, 3H), 7.68 (d, *J* = 3.2 Hz, 1H), 7.63 – 7.58 (m, 3H), 7.36 (d, *J* = 8.0 Hz, 1H), 6.97 (d, *J* = 3.2 Hz, 1H), 6.88 (d, *J* = 8.8 Hz, 2H), 6.83 (d, *J* = 8.8 Hz, 2H), 4.28 (q, *J* = 7.2 Hz, 2H), 3.88 (d, *J* = 4.8 Hz, 1H), 3.07 (s, 6H), 3.03 (s, 6H), 1.93 (s, 3H), 1.82 (d, *J* = 4.8 Hz, 1H), 1.31 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.1, 162.6, 150.7, 150.4, 144.2, 140.8, 136.3, 132.4, 130.3, 130.0, 129.5, 127.7, 127.5, 127.2, 126.1 (t, *J* = 9.7 Hz), 125.8, 125.5, 124.2, 123.3, 119.4, 112.7, 112.3, 111.0, 104.8, 61.9, 40.5, 40.4, 31.7, 30.8, 30.0, 16.9, 14.3. HRMS (ESI) m/z: Calcd for $C_{38}H_{38}BN_4O_2F_2$ $[M+H]^+$ 631.3056; Found 631.3081.

3. Nomorlized Absorption and Fluorescent Spectra of BF_2 Complexes.

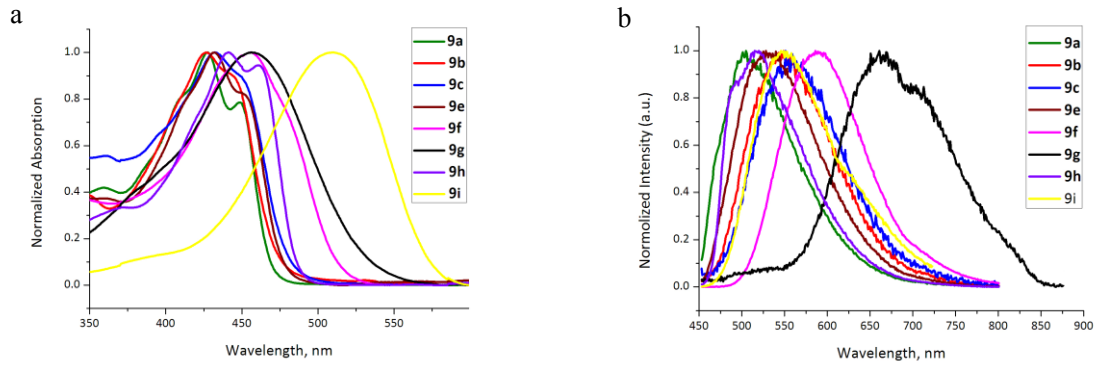


Figure S1. Nomorlized absorption (a) and fluorescent spectra (b) of BF_2 complexes.

4. Quantum Yield Calculation of BF_2 Complexes.

DCM (4-(Dicyanomethylene)-2-methyl-6-(4-dimethylaminostyryl)-4H-pyran) was chosen as a reference compound for the determination of quantum yield. Quantum yields of the standard sample: ϕ_{DCM_443nm}= 0.44, ϕ_{DCM_520nm}= 0.45. The quantum yield was calculated using the following equation:

$$\phi_U = \phi_S \frac{Grad_U}{Grad_S} \frac{n_u^2}{n_s^2}$$

Where ϕ is the fluorescence quantum yield, *Grad* is the gradient from the plot of integrated fluorescence intensity vs. absorbance. Subscripts S and U refer to the standard and to the unknown, respectively. For compounds **9a-c** and **9e-h**, the excitation wavelength is at 443 nm; for compound **9i**, the excitation wavelength is at 520 nm.

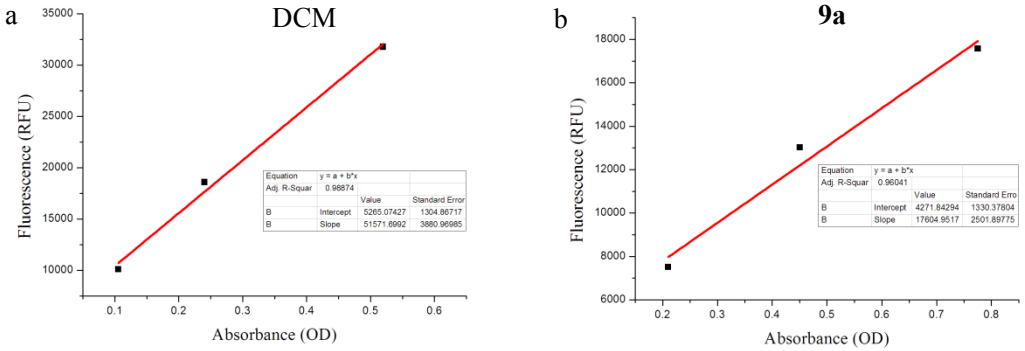


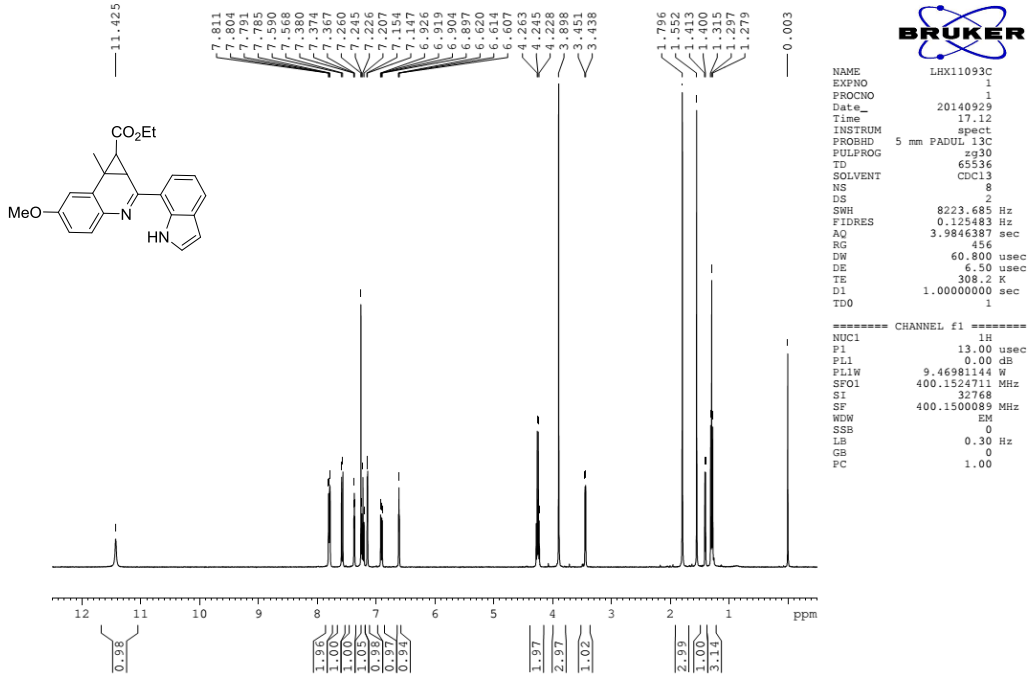
Figure S2. Linear plots of standard sample a (DCM) and test samples b (**9a**) in dichloromethane. Conditions: excitation wavelength = 443 nm.

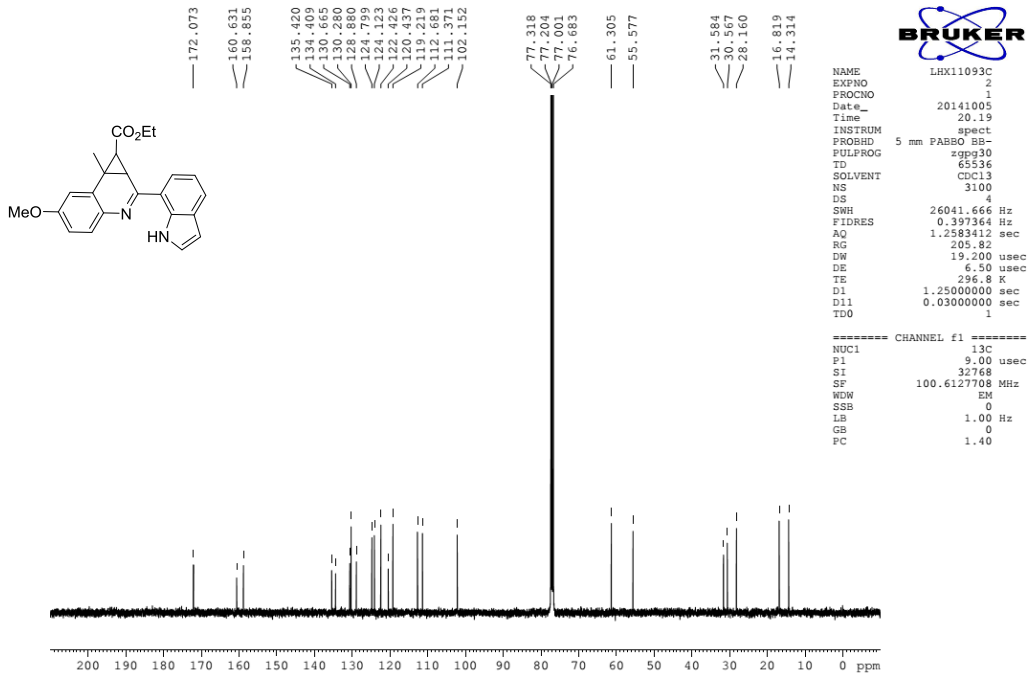
$$\phi_{9a} = 0.44 \frac{17605}{51572} \frac{1.333^2}{1.333^2} = 0.15$$

The other fluorescence quantum yield is caculated in accordance with **9a**.

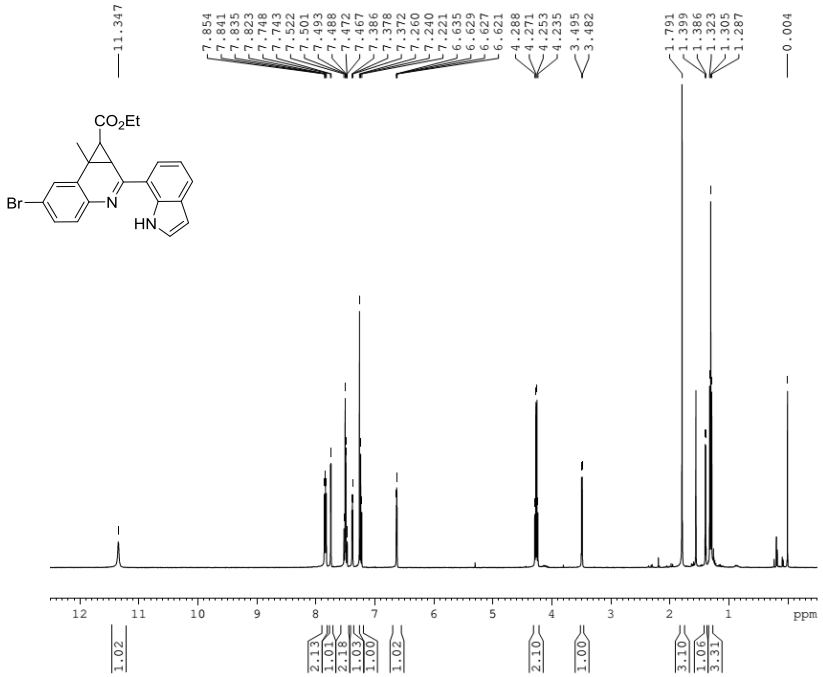
5. NMR Spectra.

^{1}H NMR ($CDCl_3$, 400 MHz) and ^{13}C NMR ($CDCl_3$, 100 MHz) spectra of **8a**





^{1}H NMR ($CDCl_3$, 400 MHz) and ^{13}C NMR ($CDCl_3$, 100 MHz) spectra of **8b**



BRUKER

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PROCNO                    1
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PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                        8
DS                        0
SWH                8223.685 Hz
FIDRES             0.125483 Hz
AQ                 3.9846387 sec
RG                    205.82
DW                  60.800 usec
DE                   6.50 usec
TE                   296.0 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     1H
P1                  14.00 usec
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SF           400.1300103 MHz
WDW                      EM
SSB                       0
LB                   0.30 Hz
GB                        0
PC                     1.00
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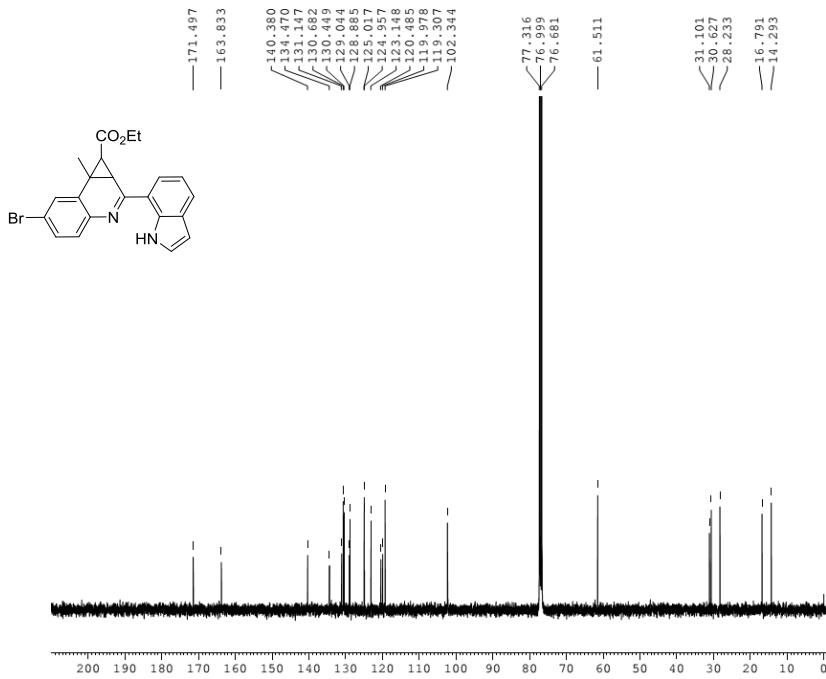

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PROCNO                    1
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TD                    65536
SOLVENT               CDCl3
NS                      817
DS                        4
SWH               26041.666 Hz
FIDRES             0.397364 Hz
AQ                 1.2583412 sec
RG                    205.82
DW                  19.200 usec
DE                   6.50 usec
TE                   296.6 K
D1                1.25000000 sec
D11               0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    13C
P1                   9.00 usec
SI                    32768
SF           100.6127716 MHz
WDW                      EM
SSB                       0
LB                   1.00 Hz
GB                        0
PC                     1.40
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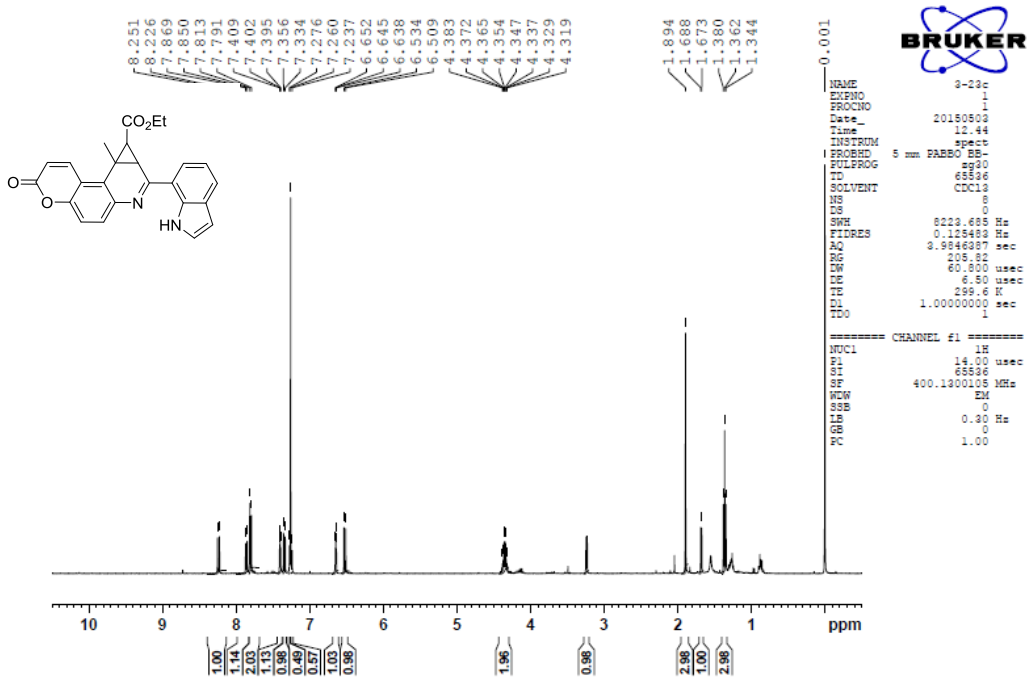
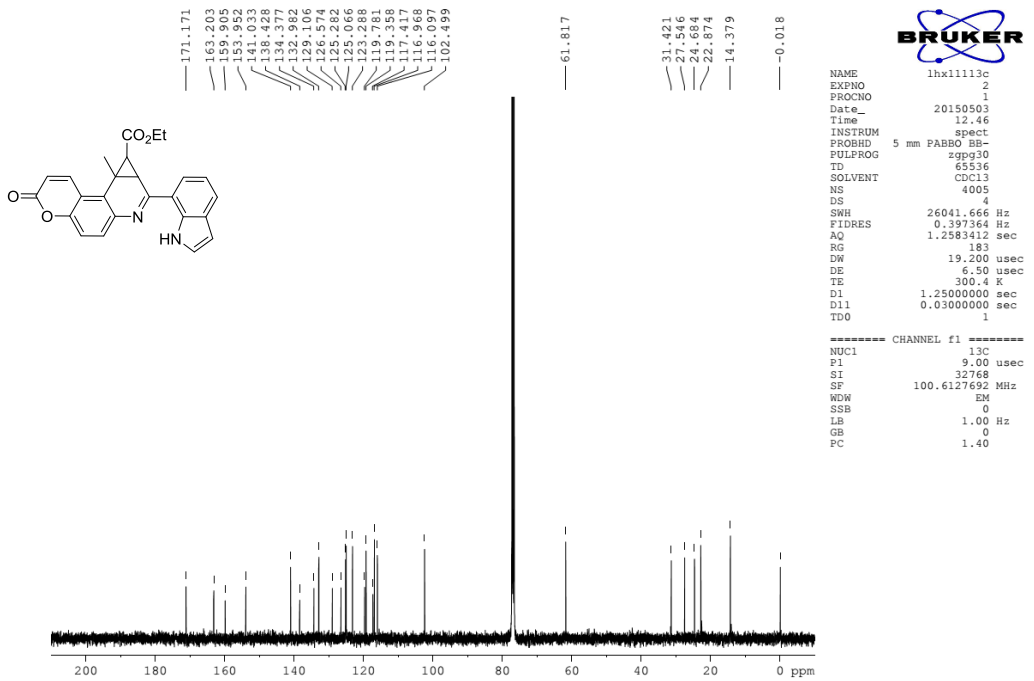
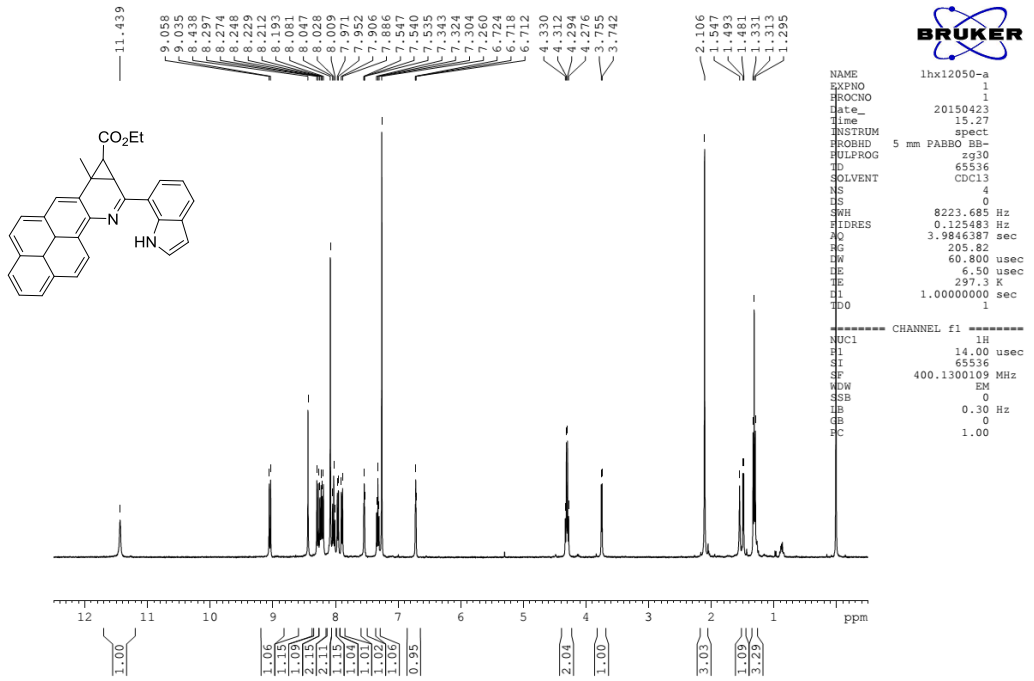
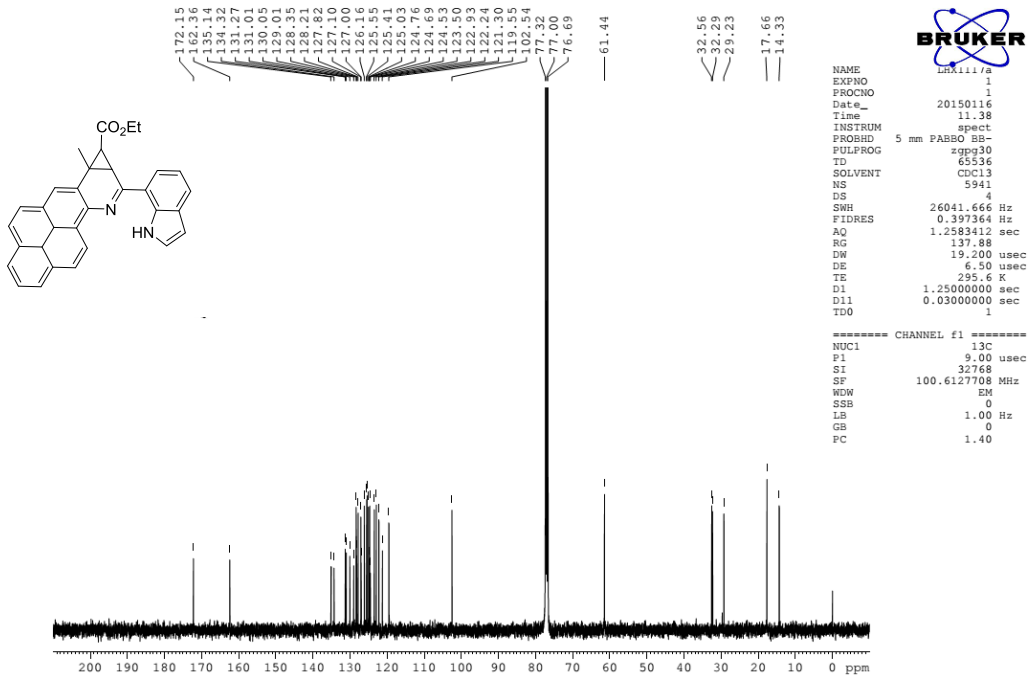
^{1}H NMR ($CDCl_3$, 400 MHz) and ^{13}C NMR ($CDCl_3$, 100 MHz) spectra of **8c**



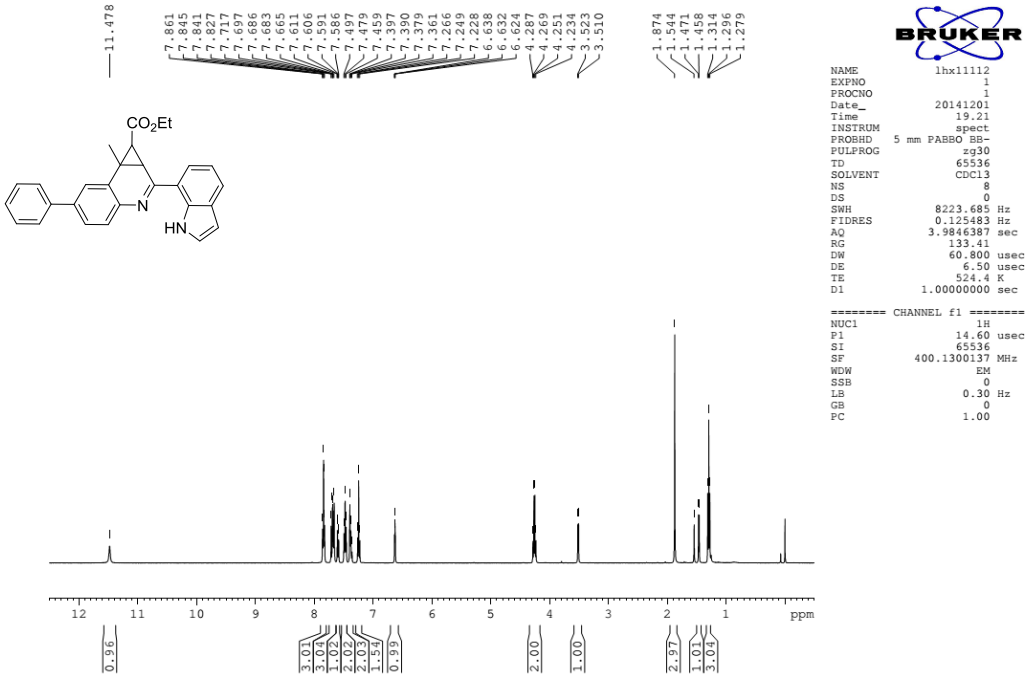


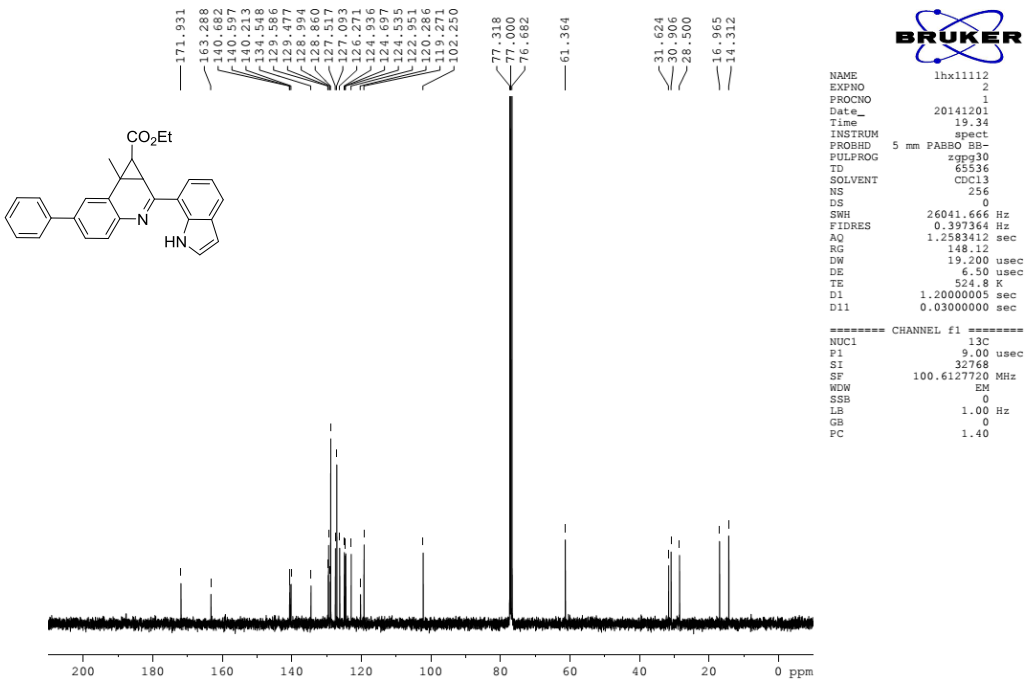
^{1}H NMR ($CDCl_3$, 400 MHz) and ^{13}C NMR ($CDCl_3$, 100 MHz) spectra of **8d**



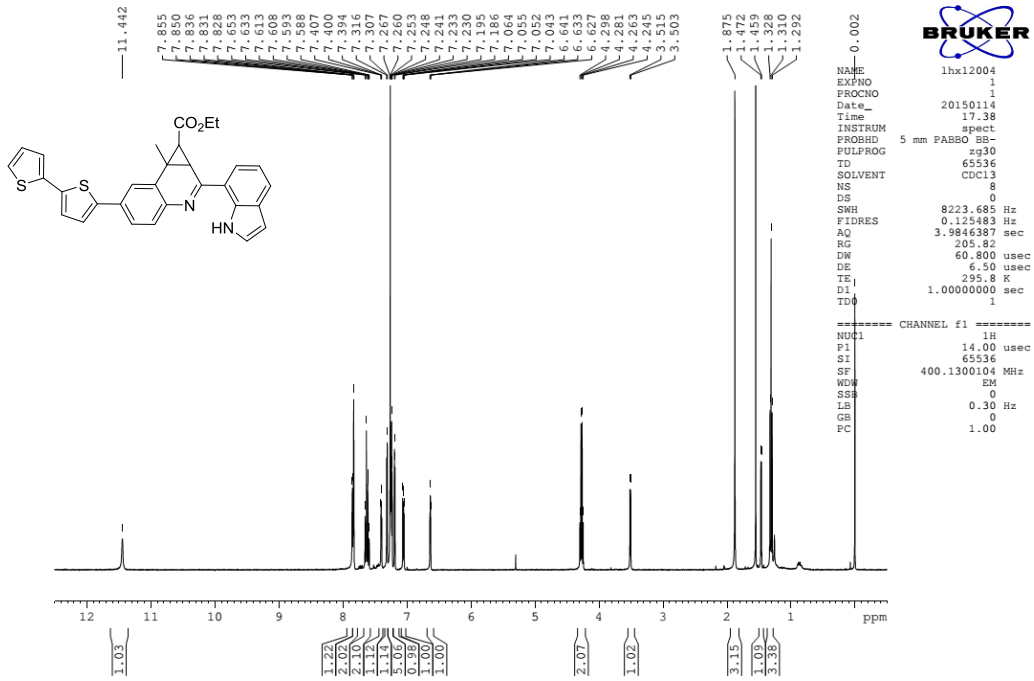


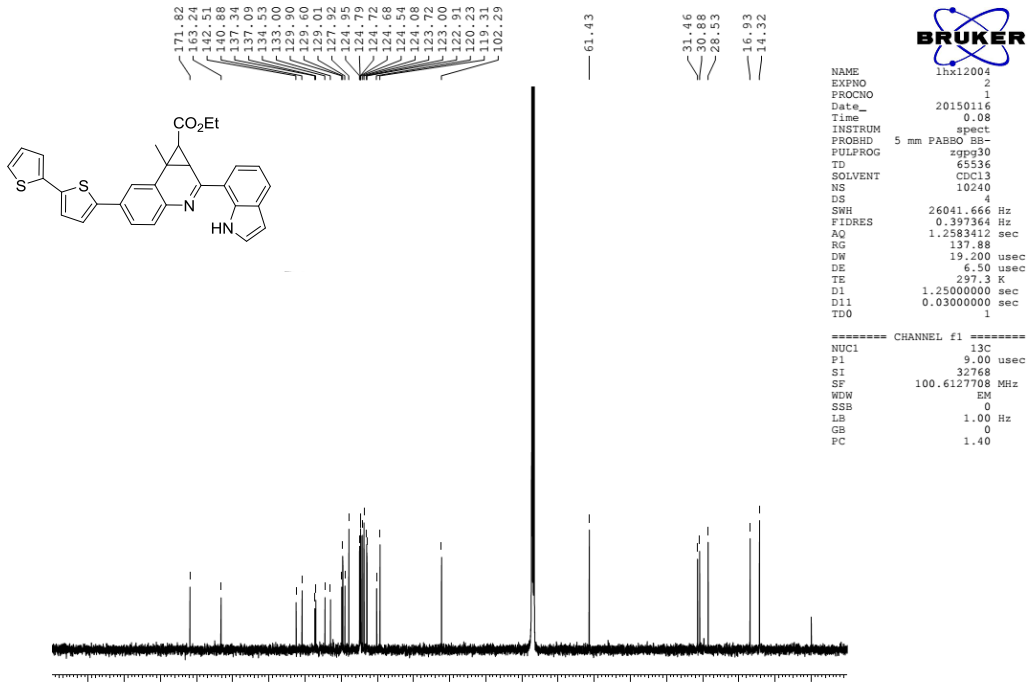
^{1}H NMR ($CDCl_3$, 400 MHz) and ^{13}C NMR ($CDCl_3$, 100 MHz) spectra of **8e**



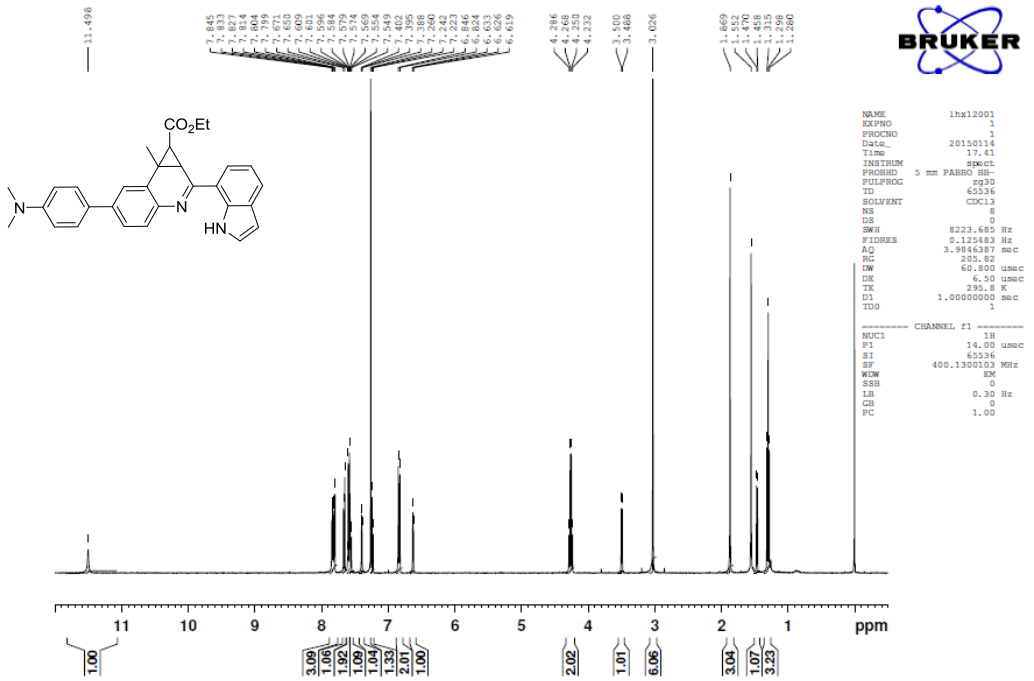


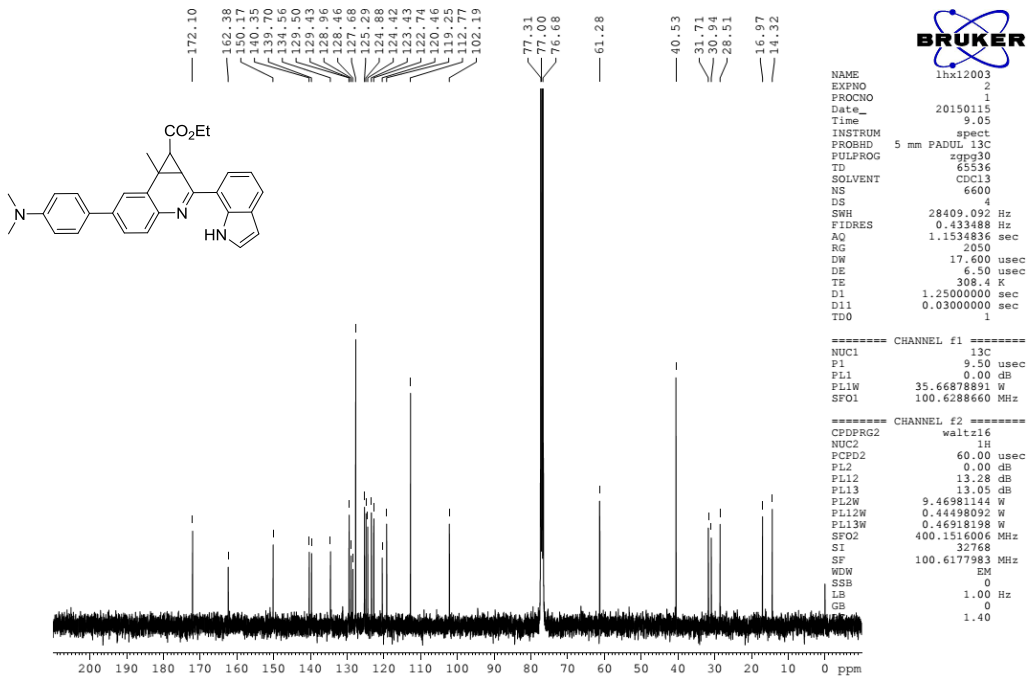
^{1}H NMR ($CDCl_3$, 400 MHz) and ^{13}C NMR ($CDCl_3$, 100 MHz) spectra of **8f**



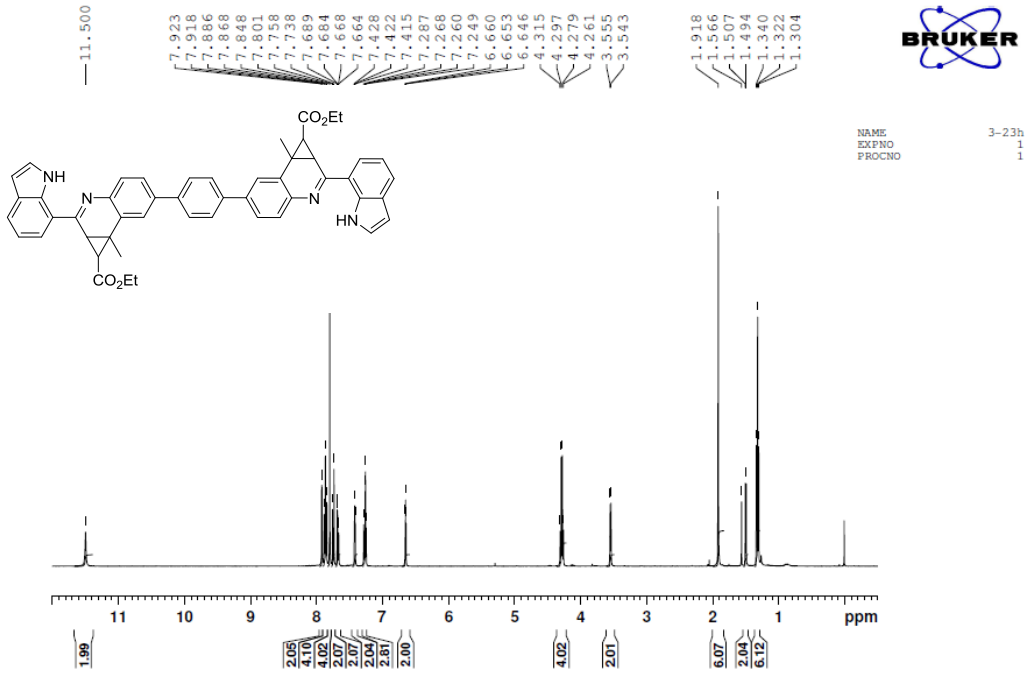


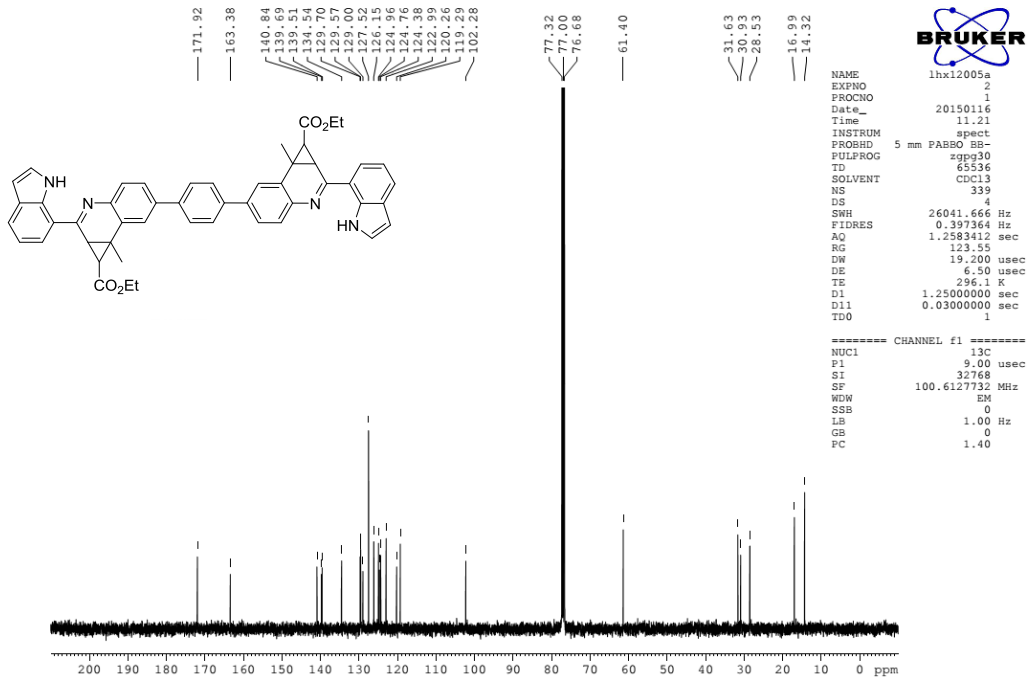
^{1}H NMR ($CDCl_3$, 400 MHz) and ^{13}C NMR ($CDCl_3$, 100 MHz) spectra of **8g**



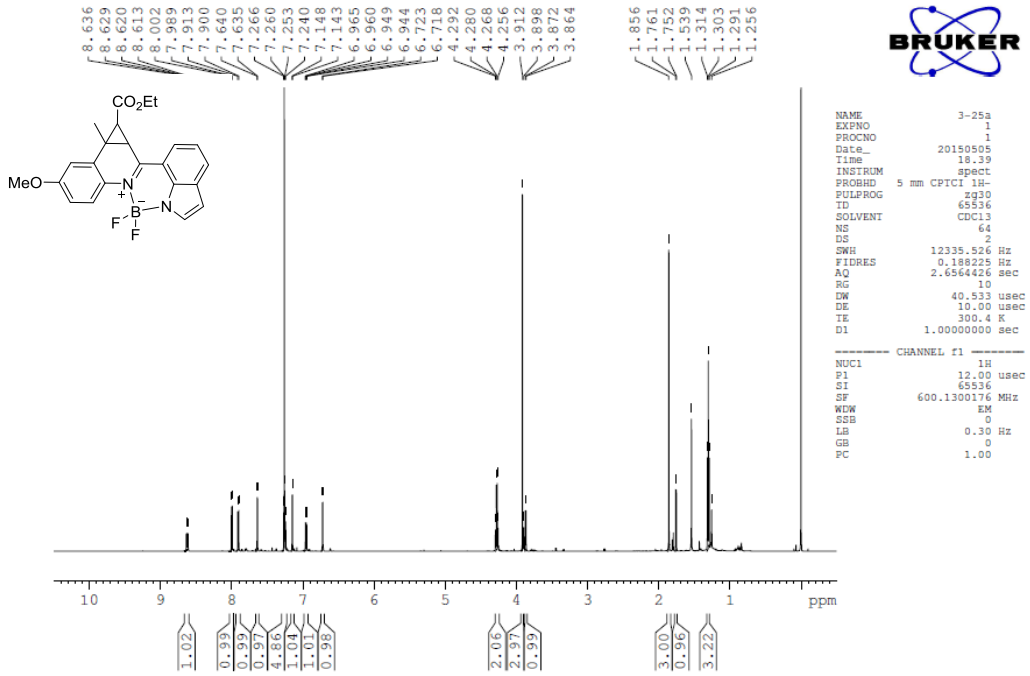


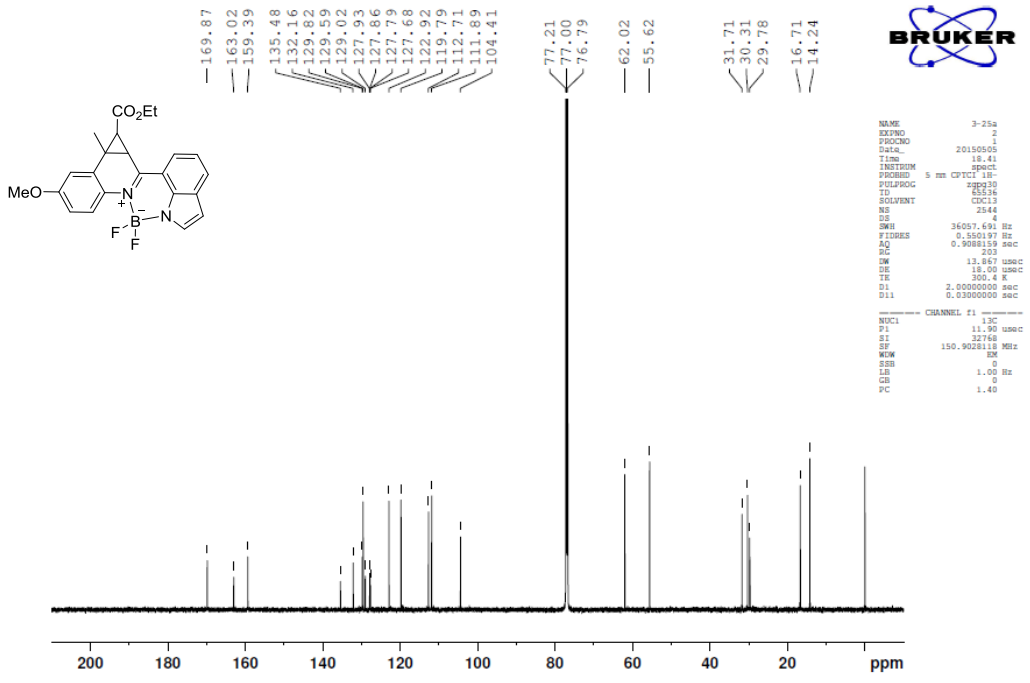
^{1}H NMR ($CDCl_3$, 400 MHz) and ^{13}C NMR ($CDCl_3$, 100 MHz) spectra of **8h**



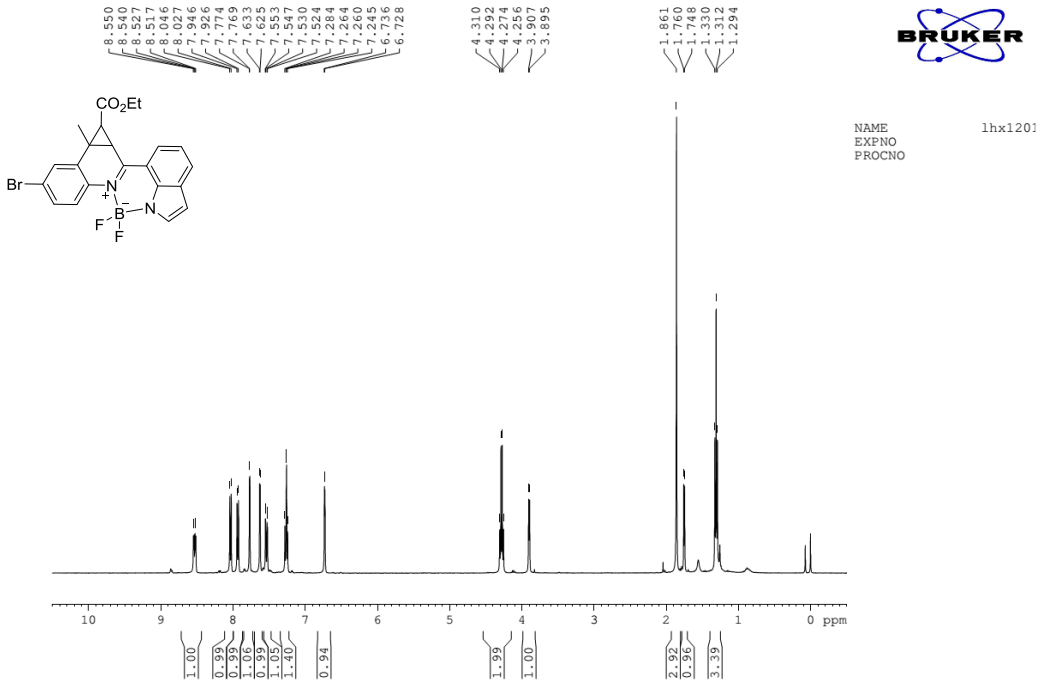


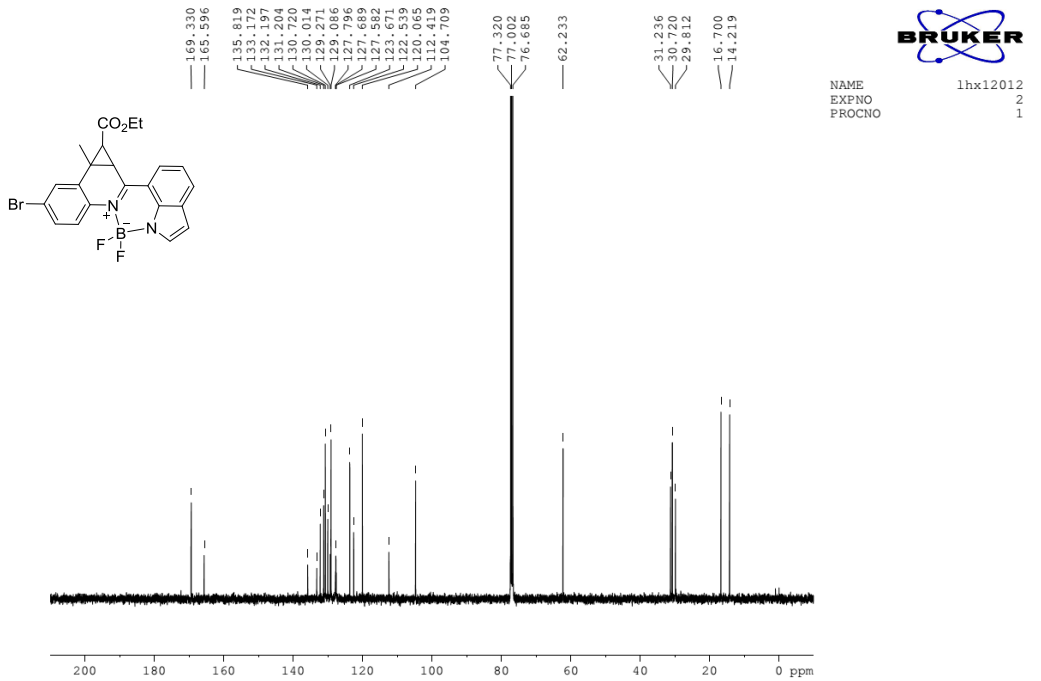
^{1}H NMR ($CDCl_3$, 600 MHz) and ^{13}C NMR ($CDCl_3$, 150 MHz) spectra of **9a**



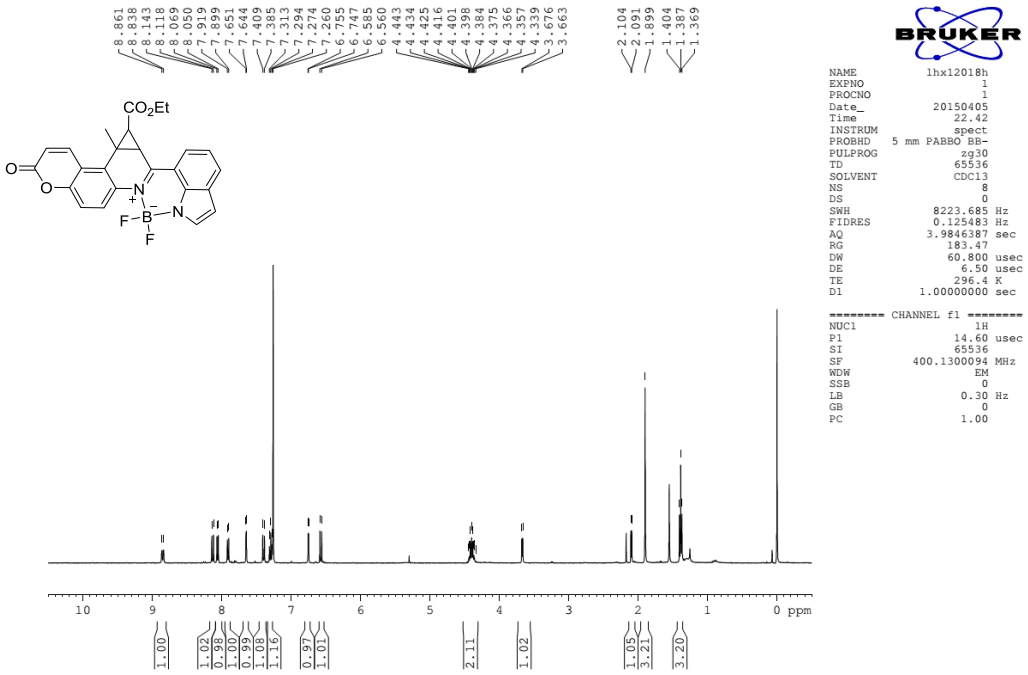


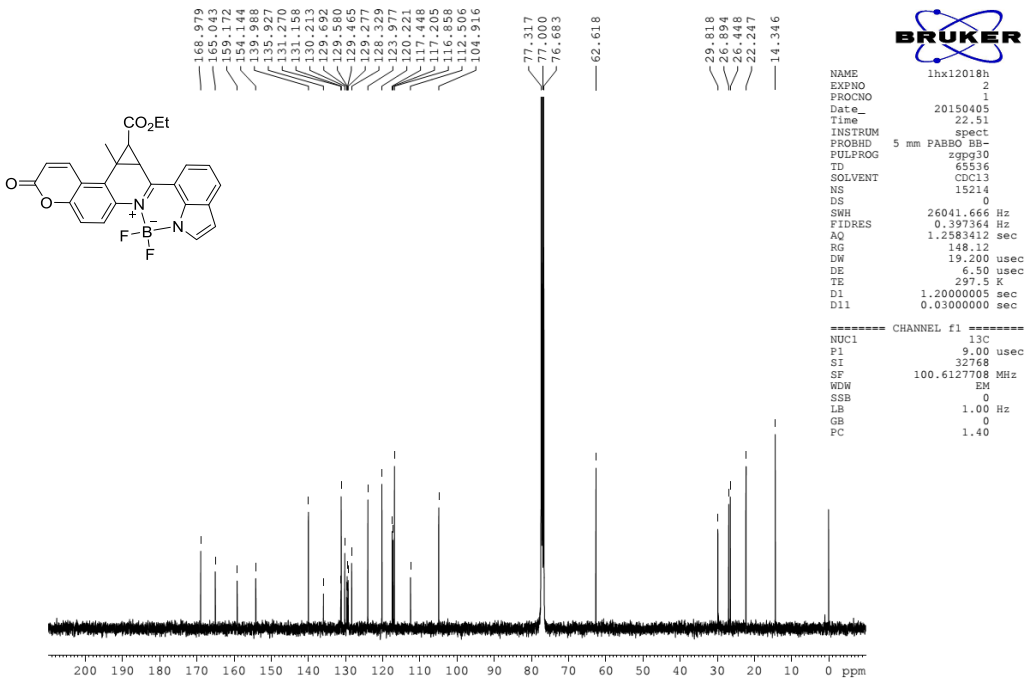
^{1}H NMR ($CDCl_3$, 400 MHz) and ^{13}C NMR ($CDCl_3$, 100 MHz) spectra of **9b**



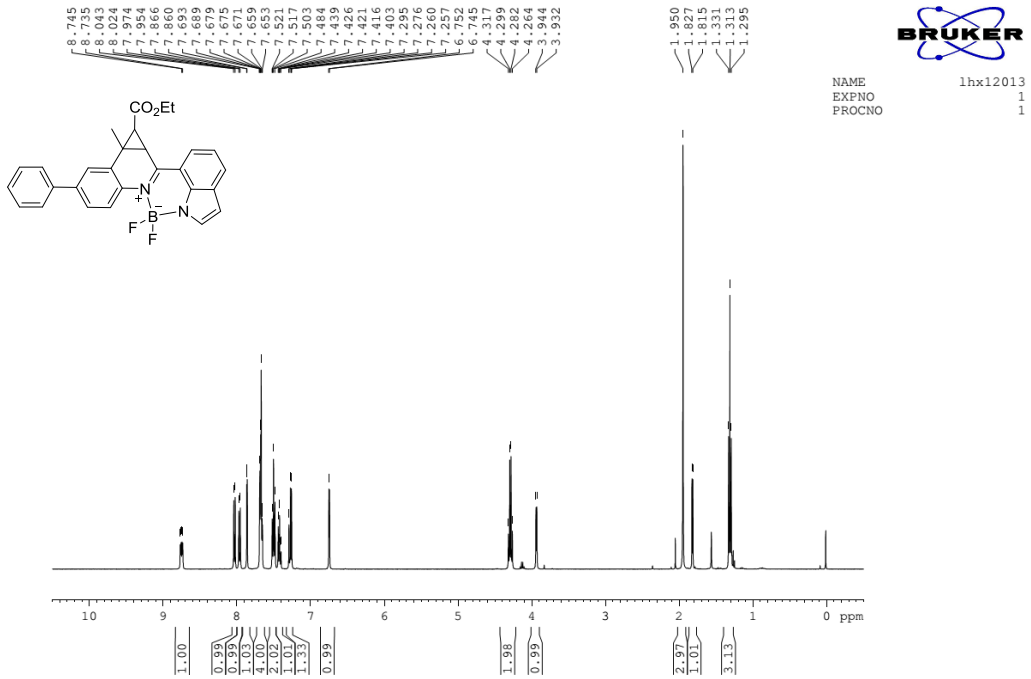


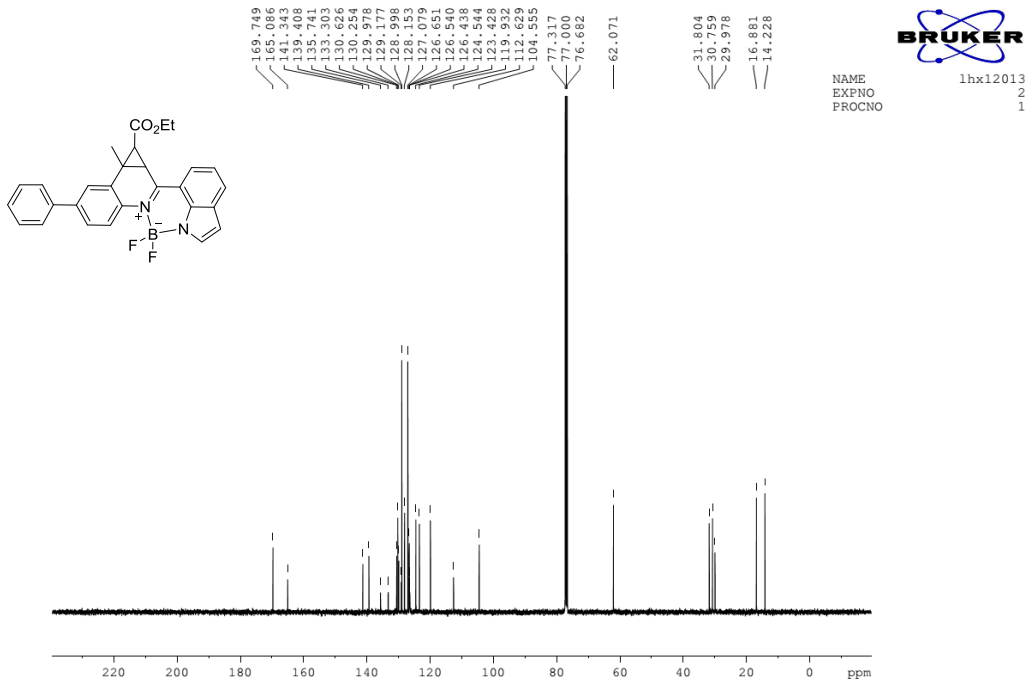
^{1}H NMR ($CDCl_3$, 400 MHz) and ^{13}C NMR ($CDCl_3$, 100 MHz) spectra of **9c**



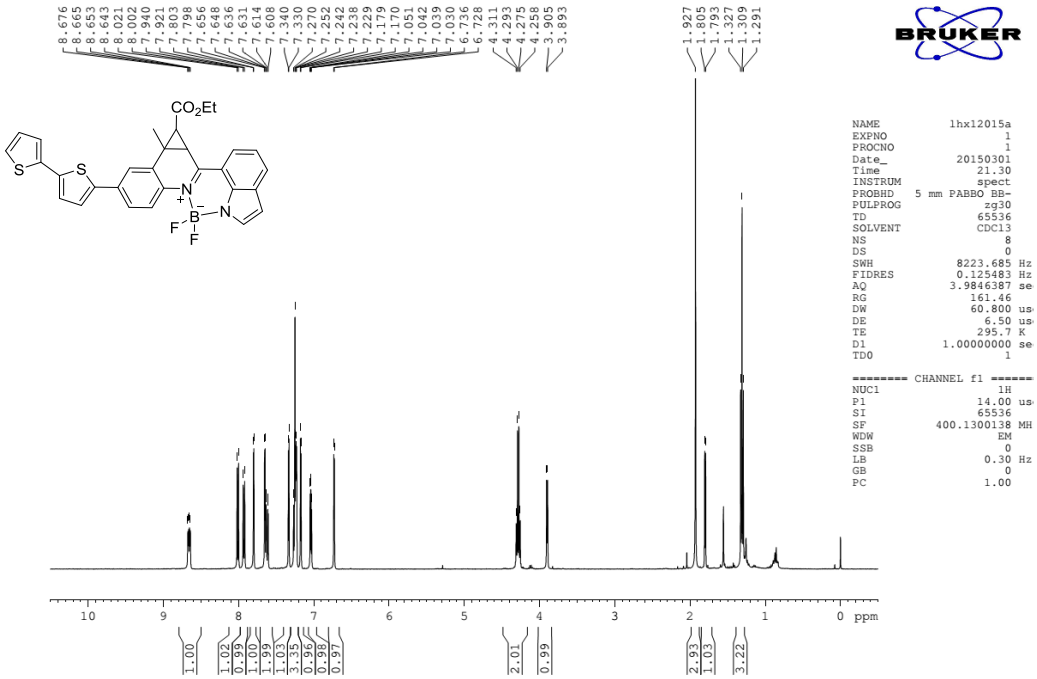


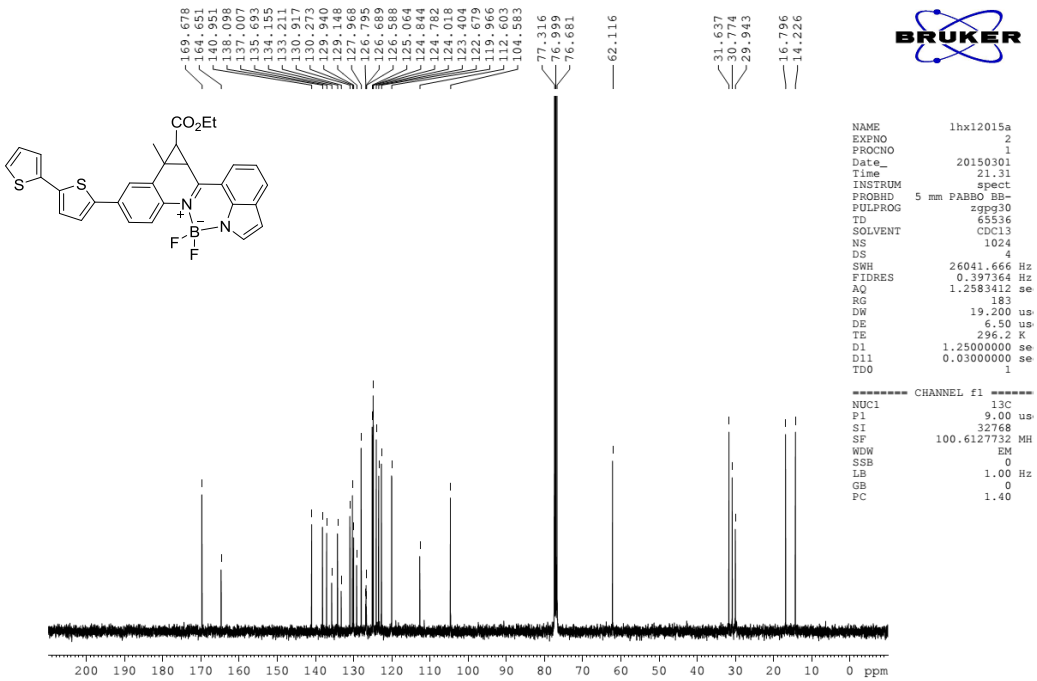
^{1}H NMR ($CDCl_3$, 400 MHz) and ^{13}C NMR ($CDCl_3$, 100 MHz) spectra of **9e**



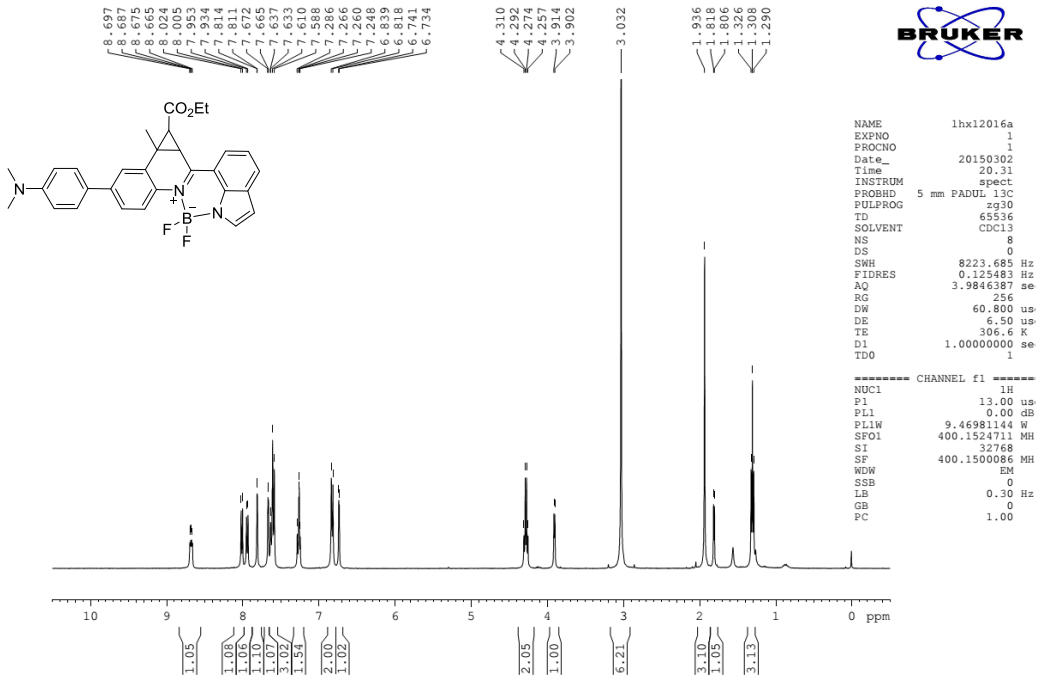


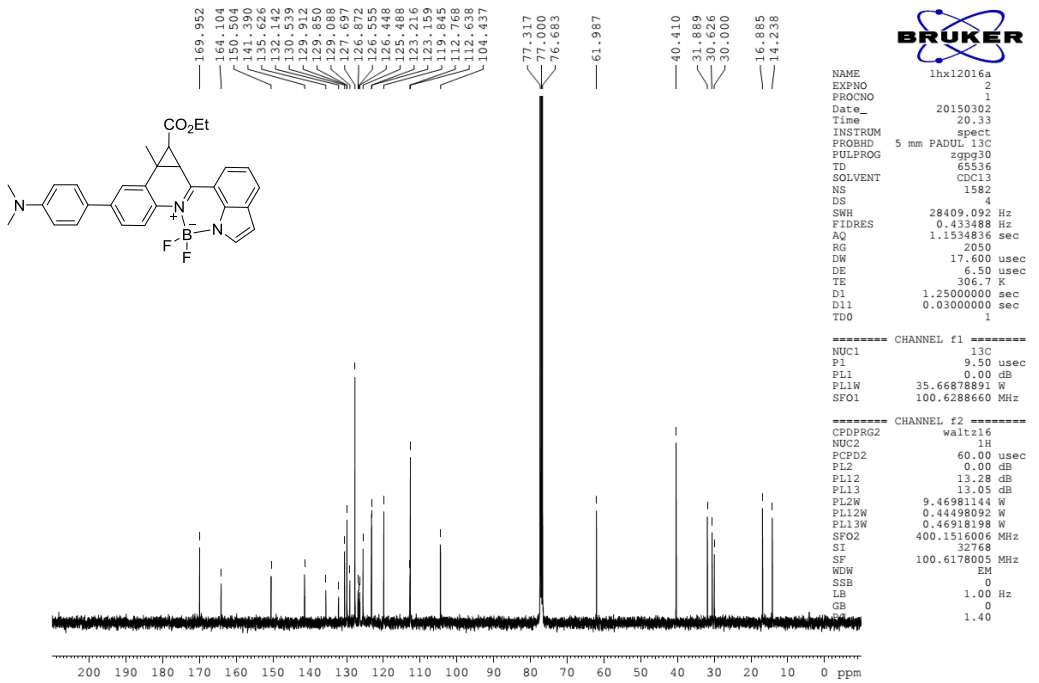
^{1}H NMR ($CDCl_3$, 400 MHz) and ^{13}C NMR ($CDCl_3$, 100 MHz) spectra of **9f**



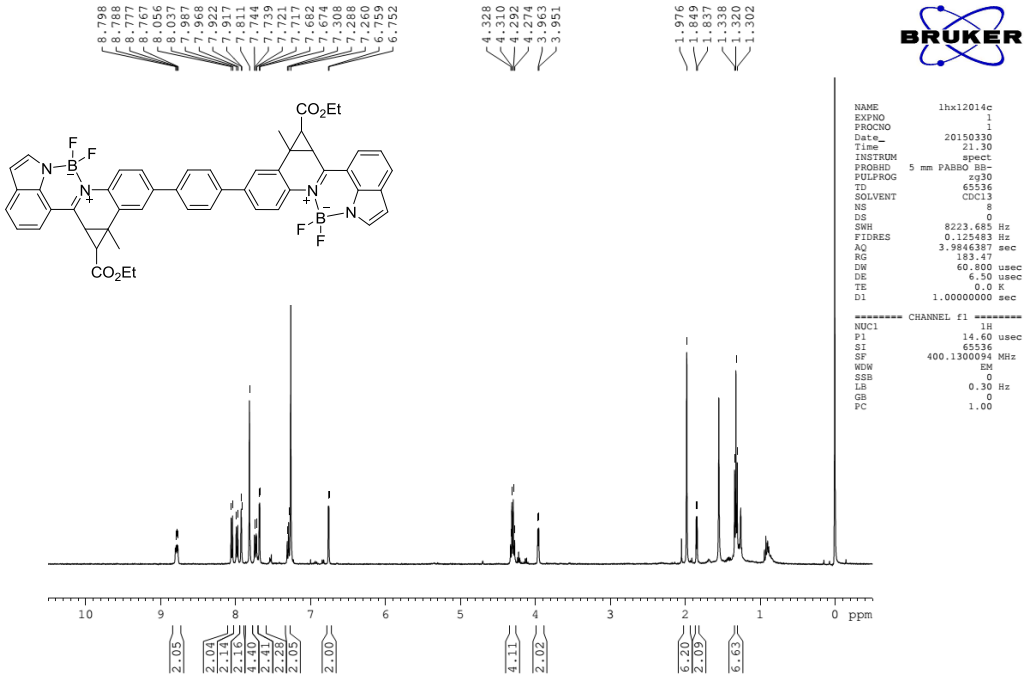


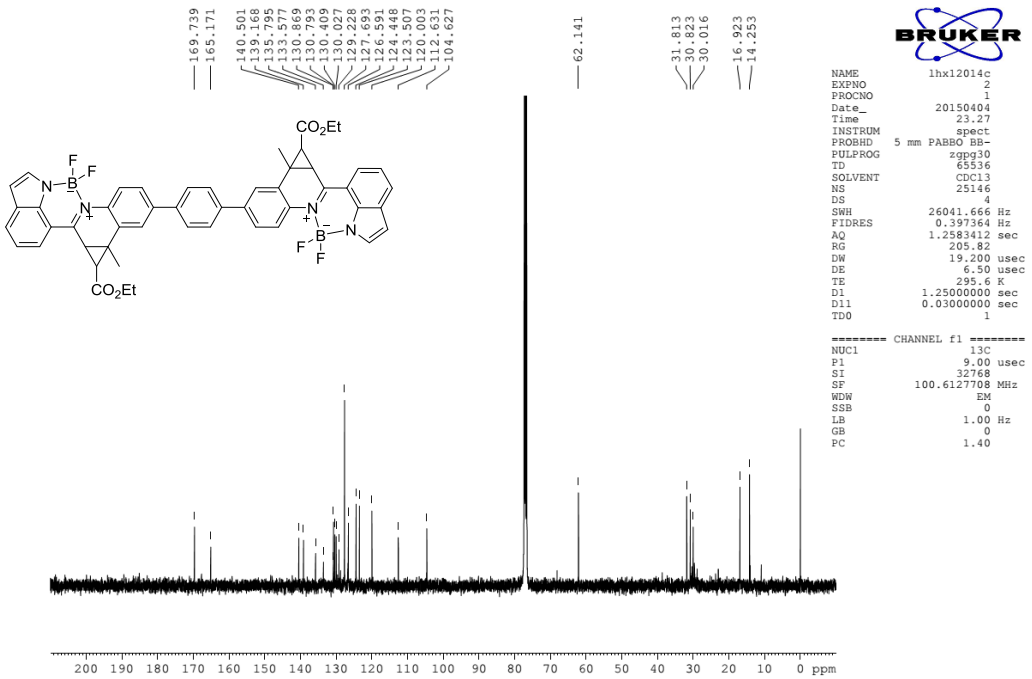
^{1}H NMR ($CDCl_3$, 400 MHz) and ^{13}C NMR ($CDCl_3$, 100 MHz) spectra of **9g**



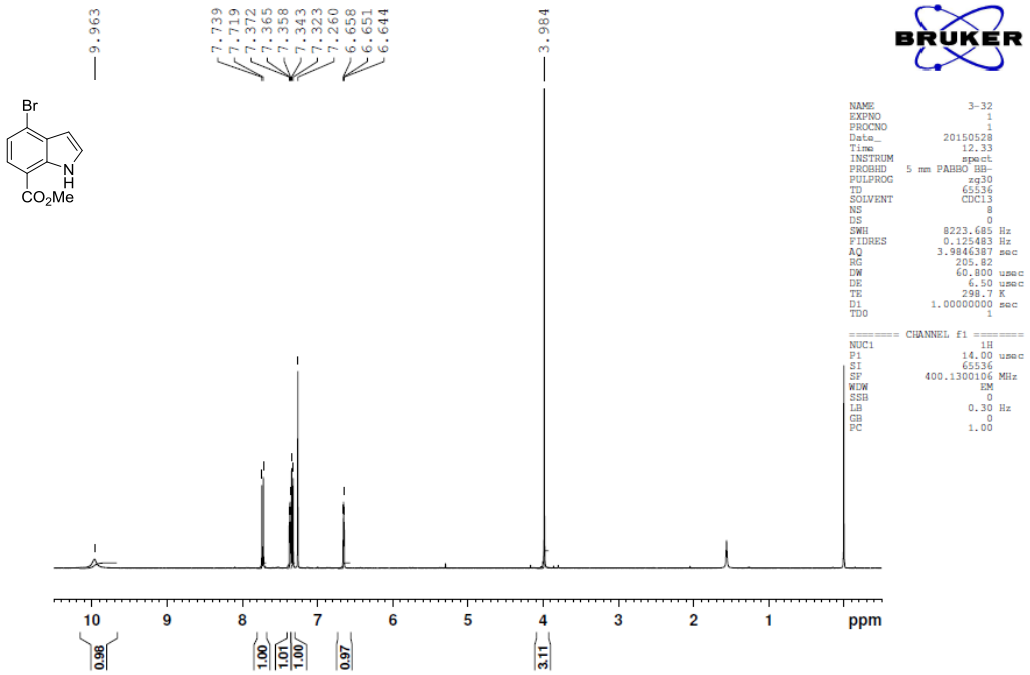


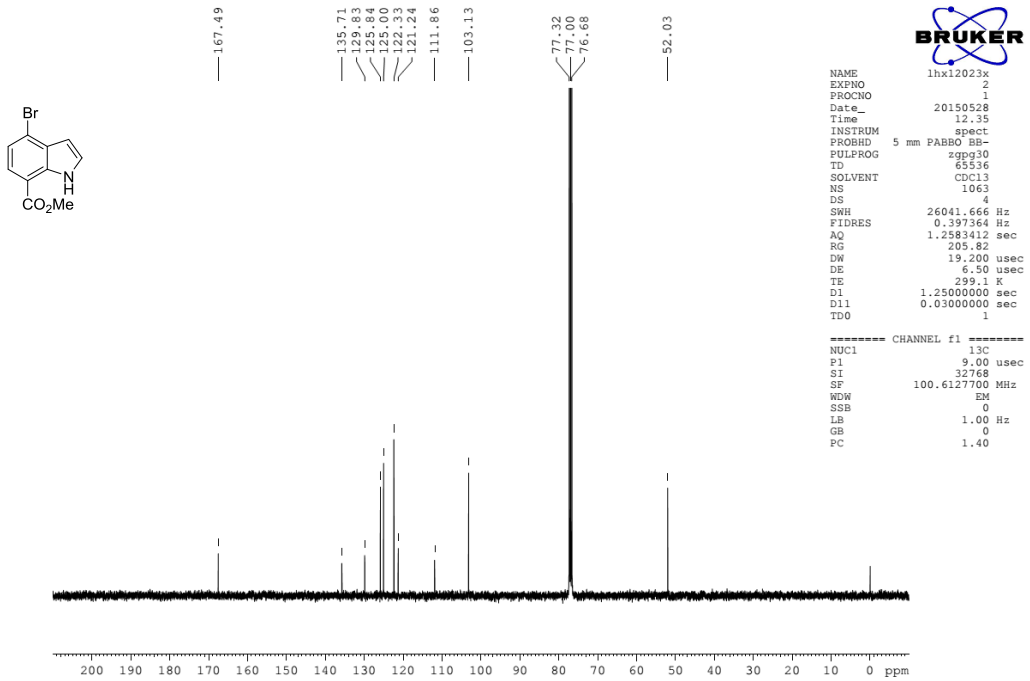
^{1}H NMR ($CDCl_3$, 400 MHz) and ^{13}C NMR ($CDCl_3$, 100 MHz) spectra of **9h**



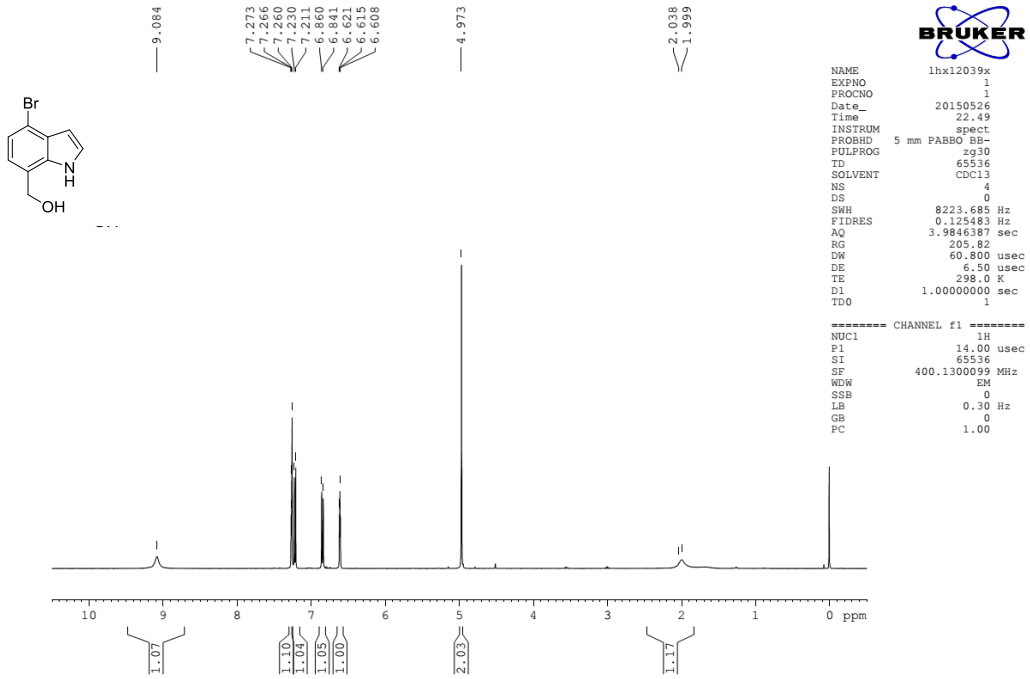


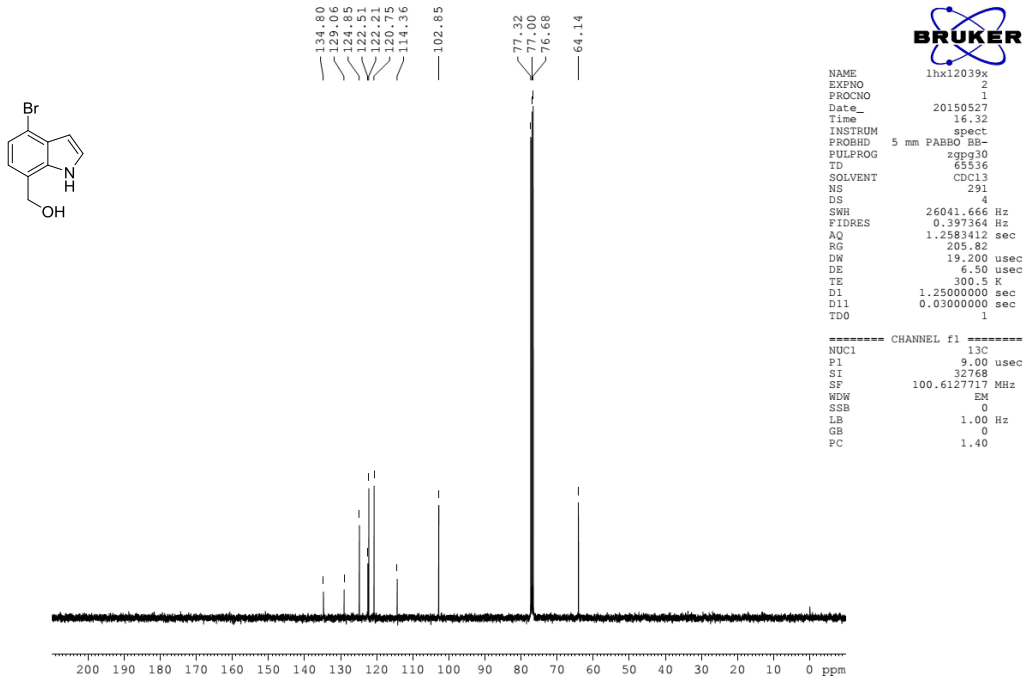
^{1}H NMR ($CDCl_3$, 400 MHz) and ^{13}C NMR ($CDCl_3$, 100 MHz) spectra of **13**



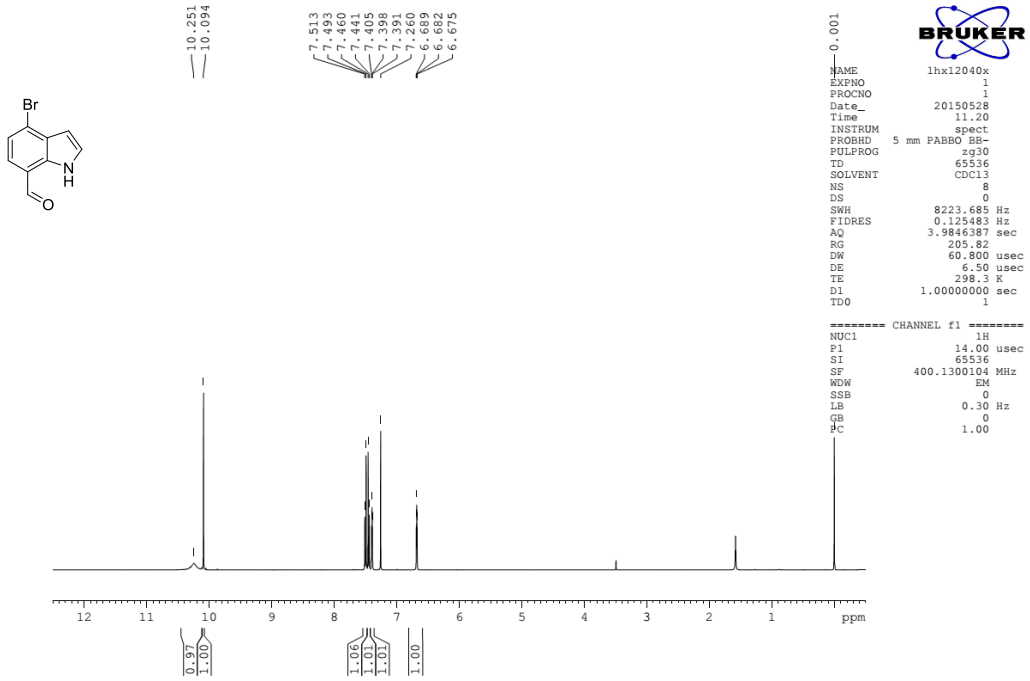


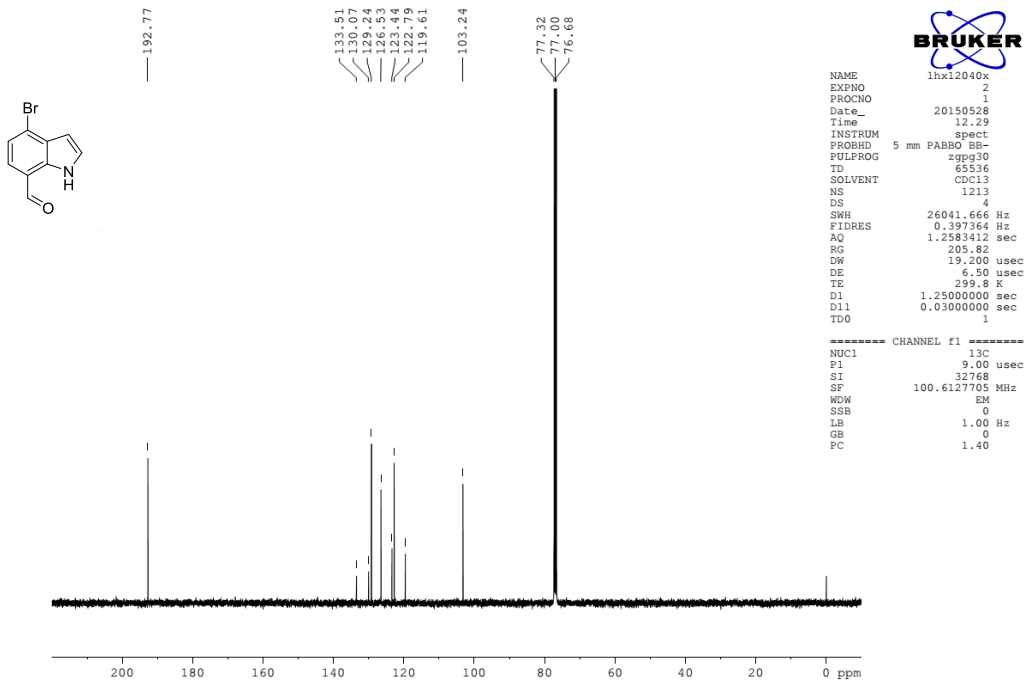
^{1}H NMR ($CDCl_3$, 400 MHz) and ^{13}C NMR ($CDCl_3$, 100 MHz) spectra of **14**



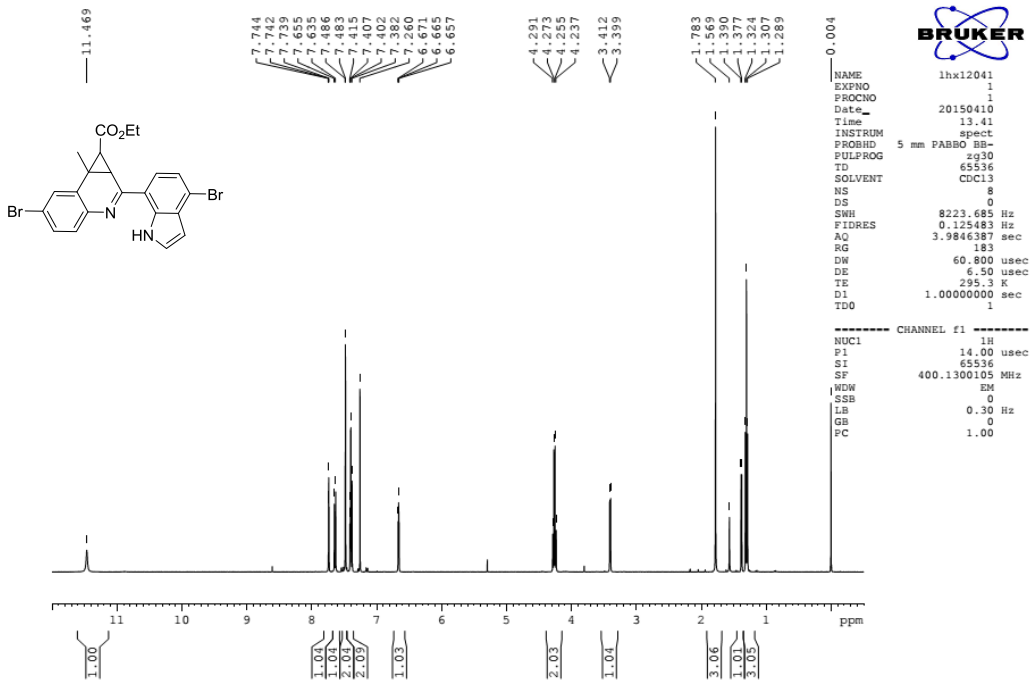


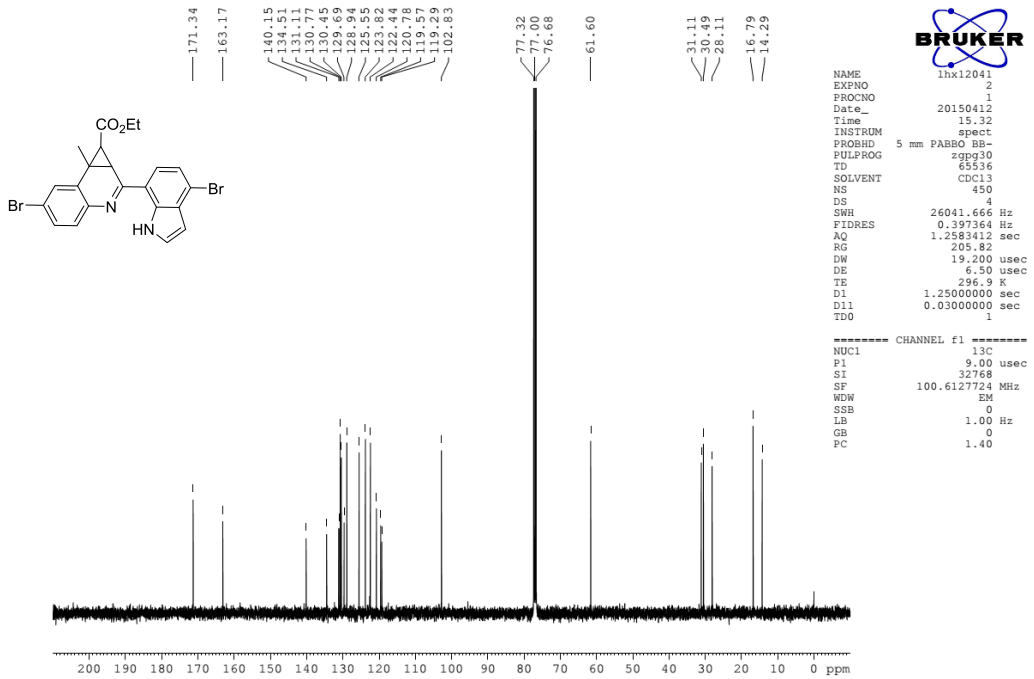
^{1}H NMR ($CDCl_3$, 400 MHz) and ^{13}C NMR ($CDCl_3$, 100 MHz) spectra of **15**



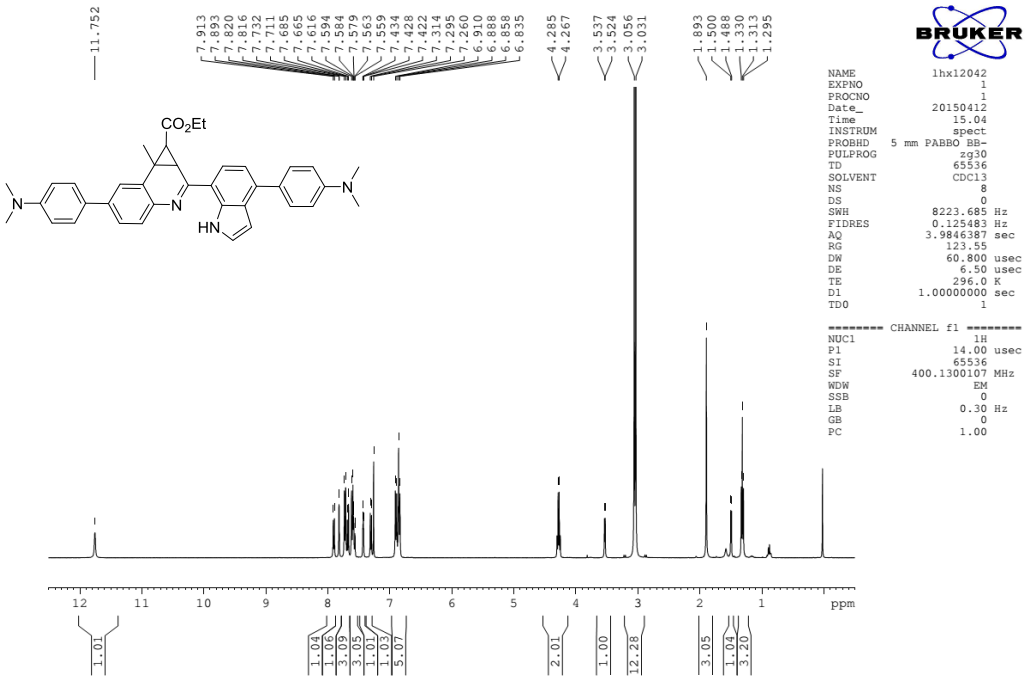


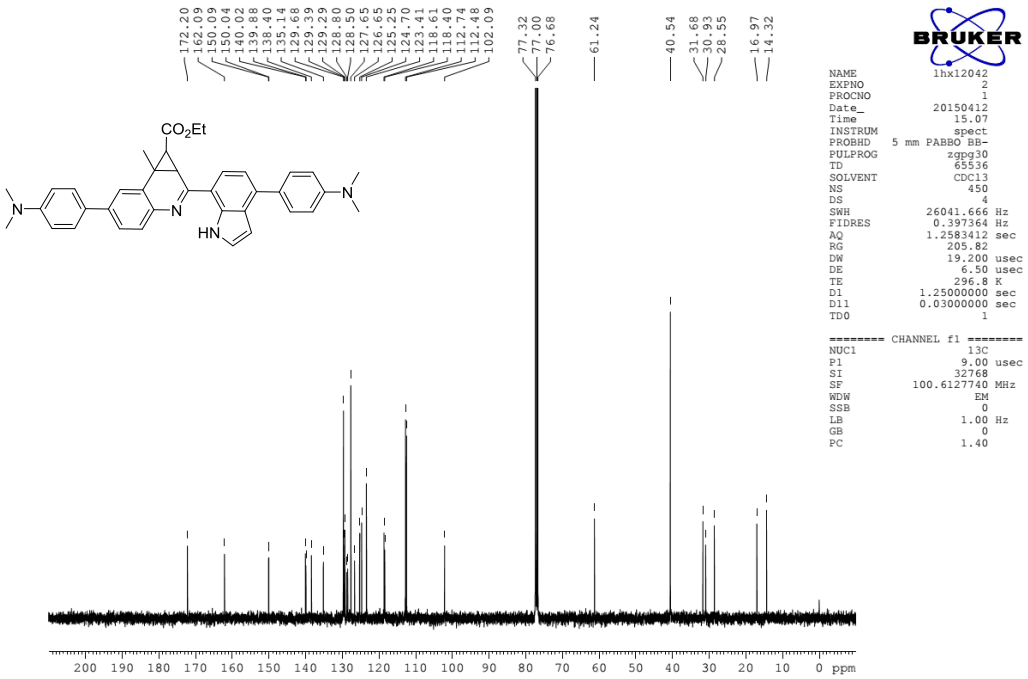
^{1}H NMR ($CDCl_3$, 400 MHz) and ^{13}C NMR ($CDCl_3$, 100 MHz) spectra of **8j**



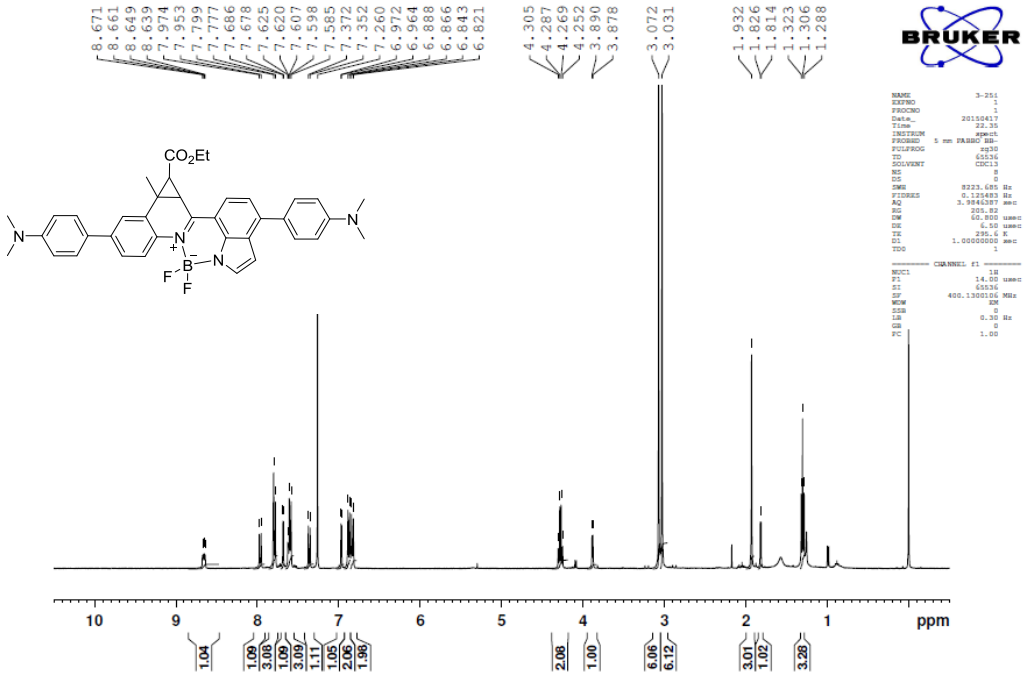


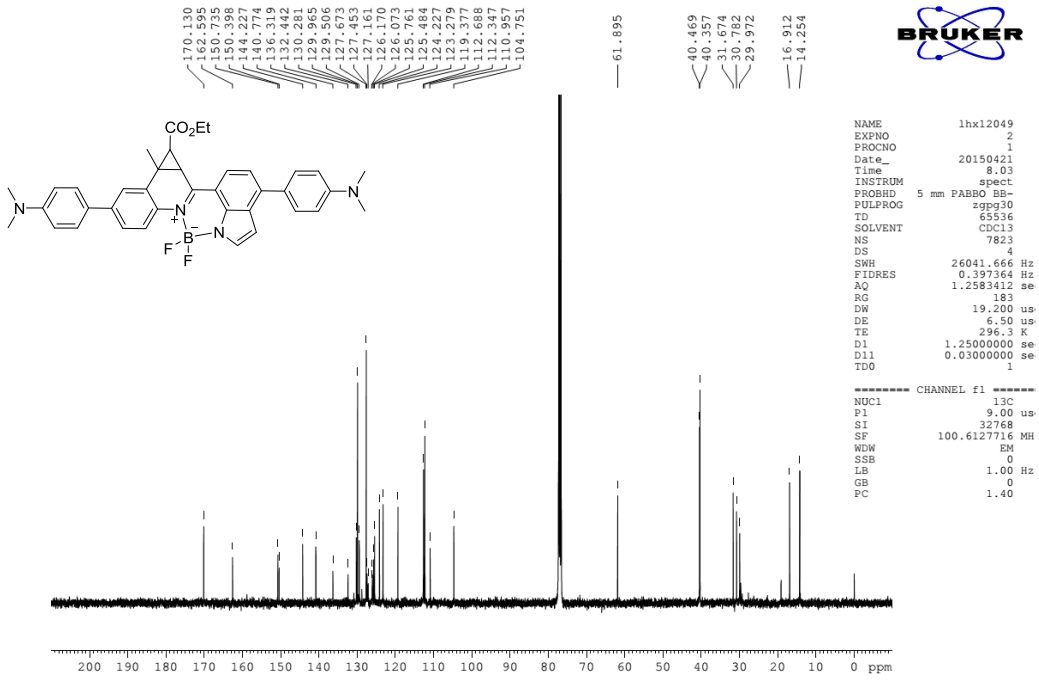
^{1}H NMR ($CDCl_3$, 400 MHz) and ^{13}C NMR ($CDCl_3$, 100 MHz) spectra of **8i**





^{1}H NMR ($CDCl_3$, 400 MHz) and ^{13}C NMR ($CDCl_3$, 100 MHz) spectra of **9i**





6. Reference:

1. Gaussian 09, Revision A.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar,J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.