

## *Electronic Supplementary Information*

### **Study on the solution and solid-state fluorescence of novel BF<sub>2</sub> complexes with (*Z*)-2-[phenanthridin-6(*5H*)-ylidene]-1-phenylethanone and its derivatives as ligands**

Ding-Er Wu, Xiao-Lin Lu and Min Xia\*

Department of Chemistry, Zhejiang Sci-Tech University, Hangzhou 310018, P. R. China

E-mail: xiamin@zstu.edu.cn

#### **Materials and measurements**

All the reagents used were analytically pure and some chemicals were further purified by recrystallization or distillation. Melting points were determined by an OptiMelt automated melting point system. The <sup>1</sup>H (400 MHz) and <sup>13</sup>C NMR (100 MHz) spectra were obtained on a Bruker Avance II DMX400 spectrometer using DMSO-d<sub>6</sub> or CDCl<sub>3</sub> as the solvent and tetramethylsilane as the internal standard. The absorption spectra were measured on a Shimadzu UV 2501(PC)S UV–Vis spectrometer and the fluorescence spectra were acquired on a Perkin-Elmer LS55 spectrophotometer. The quantum yields were measured with quinine sulfate in 0.1M sulfuric acid ( $\Phi_f=0.55$ ) or fluorescein in 0.1N NaOH ( $\Phi_f=0.91$ ) as the reference. The mass spectra were determined on a HP 1110 mass spectrometer under 70 eV attack. The single crystal structure was determined on a Bruker Gemini Ultra diffractometer with a CCD counter.

#### **Computational details**

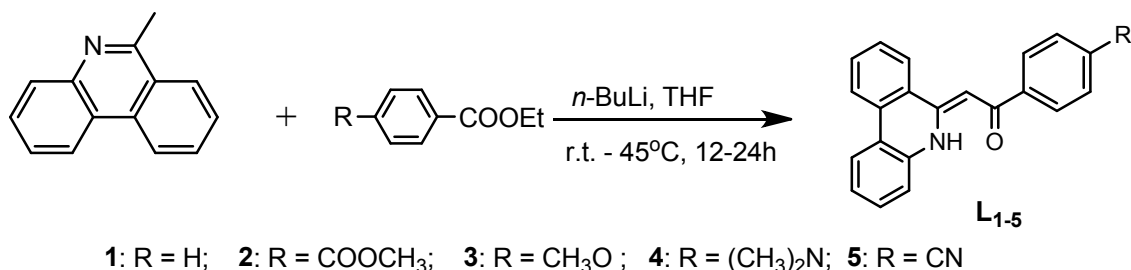
The gas-phase geometries of the concerned compounds were optimized without any symmetry restrictions in singlet ground state using the density functional theory (DFT) method at the B3LYP level. The 6–31G (d, p) basis set was selected for all the elements. The vibration frequency calculations were performed to ensure that the optimized geometries represented the global minima on the ground-state potential energy surface. All the calculations were carried out with the Gaussian 09 program package <sup>[1]</sup> in aid of the GaussView visualization program. The solvent effect was executed with the polarizable continuum model (PCM).

#### **X-ray structure analysis**

A single crystal of compounds grown in CH<sub>2</sub>Cl<sub>2</sub>/hexane mixture was selected for the X-ray analysis. The diffraction data were collected on a Bruker CCD area-detector diffractometer equipped with a graphite-

monochromated MoK $\alpha$  radiation ( $\lambda=0.71073$  Å) at 293 K for C<sub>4</sub> and 171 K for C<sub>6</sub>, respectively. The unit cell parameters were determined from a least-squares refinement of the setting angles. The structure was solved by direct methods and refined on  $F^2$  by the full-matrix least-squares methods with SHELXS-97. The refinement was carried out by full-matrix least squares method on the positional and anisotropic temperature parameters of the non-hydrogen atoms using SHELXL-97. All H atoms were placed in the idealized positions and constrained to ride on their parent atoms. Crystal data for compound C<sub>1</sub>: C<sub>21</sub>H<sub>14</sub>BF<sub>2</sub>NO,  $M_w = 345.14$ , orthogonal, **P n a 2<sub>1</sub>**,  $a = 30.2538(15)$  Å,  $b = 7.7754(4)$  Å,  $c = 13.4669(8)$  Å,  $\alpha = 90^\circ$ ,  $\beta = 90^\circ$ ,  $\gamma = 90^\circ$ ,  $D_{\text{calcd}} = 1.447$  g cm<sup>-3</sup>,  $Z = 8$ ,  $F(000) = 1424$ ,  $\mu = 0.104$  mm<sup>-1</sup>, 3032 reflections were corrected, 2473 unique,  $R_I = 0.0372$ ,  $wR_2 = 0.0848$ ; compound C<sub>4</sub>: C<sub>23</sub>H<sub>10</sub>BF<sub>2</sub>N<sub>2</sub>O,  $M_w = 388.21$ , orthogonal, **P b c a**,  $a = 7.2856(5)$  Å,  $b = 18.1056(11)$  Å,  $c = 27.2497(14)$  Å,  $\alpha = 90^\circ$ ,  $\beta = 90^\circ$ ,  $\gamma = 90^\circ$ ,  $D_{\text{calcd}} = 1.435$  g cm<sup>-3</sup>,  $Z = 8$ ,  $F(000) = 1616$ ,  $\mu = 0.102$  mm<sup>-1</sup>, 3284 reflections were corrected, 2426 unique,  $R_I = 0.0414$ ,  $wR_2 = 0.1039$ ; Crystallographic data for compound C<sub>1</sub> (CCDC 1011524), C<sub>4</sub> (CCDC 1010944) were deposited at CCDC center and can be obtained free of charge from The Cambridge Crystallographic Data Centre via [www.ccdc.cam.ac.uk/data\\_request/cif](http://www.ccdc.cam.ac.uk/data_request/cif).

### General procedure for the synthesis of ligand L<sub>1-5</sub>



**Scheme S1** Synthetic route to ligands L<sub>1-5</sub>

At room temperature and nitrogen atmosphere, 6-methylphenanthridine (10 mmol) in dried THF (20 mL) was added drop wise to a solution of *n*-BuLi (15 mmol) in dried THF (20 mL). After the solution was stirred for 30 min, ethyl benzoate (10 mmol) in dried THF (20 mL) was added drop wise to the above solution. The mixture was heated at 45 °C for 12-24h and the precipitate was collected by filtration. After washed with dried THF for 2-3 times, the solid was dissolved in 1% HCl aqueous solution. The solution was extracted by ether (3×10 mL) and the combined organic layer was dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>. After removal of solvent, the residue was purified on a silica-gel column chromatography with ethyl acetate/hexane as eluent.

Ligand L<sub>1</sub>: dark yellow solid, 73% yield; m.p. 127.5-128.7 °C; <sup>1</sup>H NMR(400 MHz, CDCl<sub>3</sub>) δ 6.82(s, 1H), 7.31(t,  $J=7.6$  Hz, 1H), 7.46-7.53(m, 5H), 7.60(t,  $J=7.6$  Hz, 1H), 7.71(t,  $J=7.6$  Hz, 1H), 8.05(m, 2H), 8.22(d,  $J=8$  Hz, 1H), 8.27(d,  $J=8.0$  Hz, 1H), 8.35(d,  $J=8.0$  Hz, 1H), 15.88(s, 1H); <sup>13</sup>C NMR(100 MHz, CDCl<sub>3</sub>) δ 84.85, 117.51, 119.73, 121.97, 123.03, 123.63, 124.43, 126.66, 127.48, 128.06, 129.26, 130.32, 131.36, 131.47, 134.01, 140.42, 152.15, 186.15; EI-MS (70 eV)  $m/z$ (%) 297(M<sup>+</sup>, 100), 268(55), 220(35), 192(35), 165(30), 105(60), 77(48).

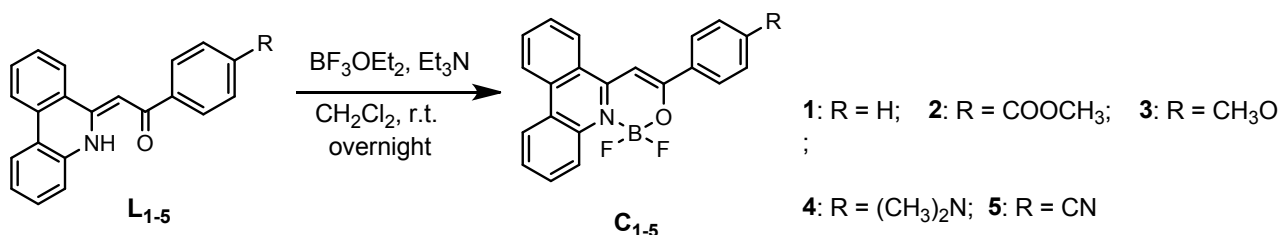
Ligand **L**<sub>2</sub>: light yellow solid, 41% yield; m.p. 206.4-207.4°C; <sup>1</sup>H NMR(400 MHz, CDCl<sub>3</sub>) δ 3.95(s, 3H), 6.76(s, 1H), 7.31(t, *J*=8 Hz, 1H), 7.44-7.52(m, 2H), 7.57(t, *J*=7.6 Hz, 1H), 7.74(t, *J*=8 Hz, 1H), 8.06(d, *J*=8 Hz, 2H), 8.12(d, *J*=8 Hz, 2H), 8.18(d, *J*=8 Hz, 1H), 8.22(d, *J*=8 Hz, 1H), 8.31(d, *J*=8 Hz, 1H), 15.94(s, 1H); <sup>13</sup>C NMR(100 MHz, CDCl<sub>3</sub>) δ 52.19, 85.69, 118.31, 120.46, 122.47, 122.61, 123.90, 124.07, 125.19, 126.80, 128.11, 129.62, 129.90, 131.60, 132.18, 132.22, 134.37, 144.57, 153.14, 166.71, 185.26; EI-MS (70 eV) *m/z*(%) 355(M<sup>+</sup>, 100), 326(47), 267(19), 220(50), 192(48), 165(57), 133(22), 104(27), 76(43).

Ligand **L**<sub>3</sub>: yellow solid, 87% yield; m.p. 157.2-157.8°C; <sup>1</sup>H NMR(400 MHz, CDCl<sub>3</sub>) δ 3.89(s, 3H), 6.77(s, 1H), 6.99(d, *J*=8Hz, 2H), 7.28(t, *J*=8Hz, 1H), 7.43(d, *J*=8Hz, 1H), 7.49(t, *J*=8Hz, 1H), 7.58(t, *J*=8Hz, 1H), 7.74(t, *J*=8Hz, 1H), 8.03(d, *J*=8Hz, 2H), 8.19(d, *J*=8Hz, 1H), 8.24(d, *J*=8Hz, 1H), 8.33(d, *J*=8Hz, 1H), 15.75(s, 1H); <sup>13</sup>C NMR(100 MHz, CDCl<sub>3</sub>) δ 55.3, 84.60, 113.47, 117.77, 119.96, 122.33, 122.42, 123.15, 124.33, 124.88, 127.86, 128.66, 129.67, 131.68, 131.93, 133.22, 134.64, 152.20, 161.69, 186.17; EI-MS (70 eV) *m/z*(%) 327(M<sup>+</sup>, 96), 312(11), 299(37), 220(22), 192(23), 165(28), 135(100), 107(14), 92(20), 77(30).

Ligand **L**<sub>4</sub>: orange solid, 84% yield; m.p. 195.7-197.2 °C; <sup>1</sup>H NMR(400 MHz, CDCl<sub>3</sub>) δ 3.06(s, 6H), 6.75(d, *J*=8.4 Hz, 2H), 6.78(s, 1H), 7.24(t, *J*=7.6 Hz, 1H), 7.39(d, *J*=8 Hz, 1H), 7.45(t, *J*=8 Hz, 1H), 7.56(t, *J*=7.6 Hz, 1H), 7.71(t, *J*=8 Hz, 1H), 8.00(d, *J*=8.4 Hz, 2H), 8.15(d, *J*=8Hz, 1H), 8.23(d, *J*=8.4 Hz, 1H), 8.30(d, *J*=8 Hz, 1H), 15.66(s, 1H); <sup>13</sup>C NMR(100 MHz, CDCl<sub>3</sub>) δ 40.04, 84.43, 117.54, 119.75, 122.30, 122.37, 122.69, 124.73, 124.78, 127.78, 128.08, 128.58, 129.58, 131.39, 131.88, 135.05, 151.53, 152.11, 186.58; EI-MS (70 eV) *m/z*(%) 340 (M<sup>+</sup>, 100), 312(15), 148(98), 121(73), 106(10), 77(13), 42(18).

Ligand **L**<sub>5</sub>: brown solid, 93% yield; m.p. 207.5-208.4 °C; <sup>1</sup>H NMR(400 MHz, CDCl<sub>3</sub>) δ 6.68(s, 1H), 7.31(t, *J*=8 Hz, 1H), 7.44(d, *J*=8 Hz, 1H), 7.51(t, *J*=8Hz, 1H), 7.57(t, *J*=8 Hz, 1H), 7.70(d, *J*=8 Hz, 2H), 7.76(t, *J*=8 Hz, 1H), 8.05(d, *J*=8 Hz, 2H), 8.18(d, *J*=8 Hz, 2H), 8.31(d, *J*=8 Hz, 1H), 15.92(s, 1H); <sup>13</sup>C NMR(100 MHz, CDCl<sub>3</sub>) δ 85.45, 113.50, 118.37, 118.71, 120.54, 122.52, 122.67, 123.75, 124.24, 125.18, 127.31, 128.18, 129.99, 132.14, 132.22, 132.40, 134.02, 144.37, 153.28, 183.68; EI-MS (70 eV) *m/z*(%) 322(M<sup>+</sup>, 100), 293(52), 220(44), 192(34), 165(39), 130(16), 102(22).

### General procedure for the synthesis of complex **C**<sub>1-5</sub>



### Scheme S5 Synthetic route to complex C<sub>1-5</sub>

At room temperature, triethylamine (3 mmol) in dried CH<sub>2</sub>Cl<sub>2</sub> (1 mL) was added drop wise to a solution of ligand (1 mmol) in dried CH<sub>2</sub>Cl<sub>2</sub> (2 mL). After the solution was stirred for 30 min, boron trifluoride etherate (8 mmol) in dried CH<sub>2</sub>Cl<sub>2</sub> (2 mL) was added drop wise. The mixture was stirred overnight and the solvent was removed on a rotating evaporator. The residue was purified by a flash column chromatography on silica gel with dried CH<sub>2</sub>Cl<sub>2</sub> as eluent.

Complex C<sub>1</sub>: bright greenish solid, 63% yield; m.p. 201.9-206.3 °C; <sup>1</sup>H NMR(400 MHz, CDCl<sub>3</sub>) δ 7.29(s, 1H), 7.49-7.57(m, 3H), 7.63(t, *J*=8 Hz, 1H), 7.76(t, *J*=8 Hz, 2H), 7.96(t, *J*=8 Hz, 1H), 8.13(d, *J*=7.6 Hz, 2H), 8.49(d, *J*=7.6 Hz, 2H), 8.58(d, *J*=8.4 Hz, 1H), 8.85(d, *J*=8.4 Hz, 1H); EI-MS (70 eV) *m/z*(%) 345(M<sup>+</sup>, 100), 324(15), 280(47), 166(13), 159(13), 105 (12),77(25).

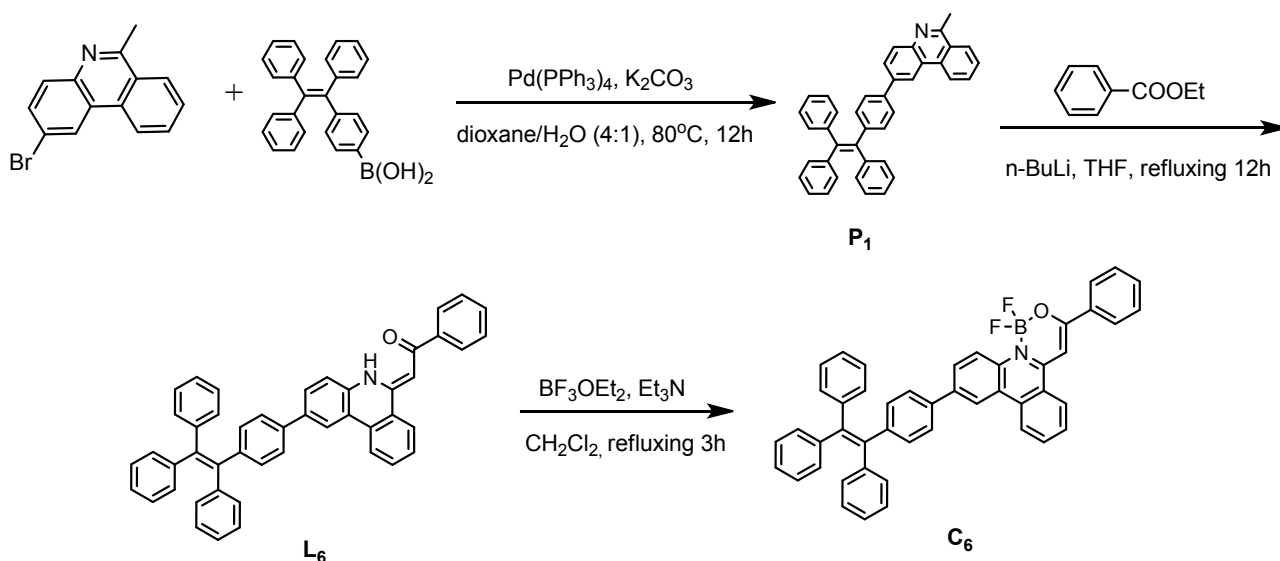
Complex C<sub>2</sub>: bright yellow solid, 81% yield; m.p. 272.8-273.5°C; <sup>1</sup>H NMR(400 MHz, CDCl<sub>3</sub>) δ 3.97(s, 3H), 7.30(s, 1H), 7.63(t, *J*=8 Hz, 1H), 7.74(d, *J*=8 Hz, 1H), 7.79(d, *J*=8 Hz, 1H), 7.98(t, *J*=8 Hz, 1H), 8.09(q, *J*=8 Hz, 4H), 8.50(t, *J*=8 Hz, 2H), 8.59(d, *J*=8 Hz, 1H), 8.84(d, *J*=8 Hz, 1H); EI-MS (70 eV) *m/z*(%) 403(M<sup>+</sup>-1, 100), 338(35), 278(18), 186(15), 139(13).

Complex C<sub>3</sub>: bright yellow solid, 76% yield; m.p. 252.5-253.5°C; <sup>1</sup>H NMR(400 MHz, CDCl<sub>3</sub>) δ 3.87(s, 1H), 6.94(d, *J*=8Hz, 2H), 7.14(s, 1H), 7.57(t, *J*=8Hz, 1H), 7.71(td, *J*<sub>1</sub>=4Hz, *J*<sub>2</sub>=8Hz, 2H), 7.91(t, *J*=8Hz, 1H), 8.04(d, *J*=8Hz, 2H), 8.44(dd, *J*<sub>1</sub>=4Hz, *J*<sub>2</sub>=8Hz, 2H), 8.53(d, *J*=8Hz, 1H), 8.77(d, *J*=8Hz, 1H); EI-MS (70 eV) *m/z*(%) 375(M<sup>+</sup>, 100), 360(11), 331(10), 310(37), 267(21), 135(16), 77(14).

Complex C<sub>4</sub>: dark red solid, 72% yield; m.p. 237.2-238.4 °C; <sup>1</sup>H NMR(400 MHz, CDCl<sub>3</sub>) δ 3.08(s, 6H), 6.72(d, *J*=8 Hz, 2H), 7.09(s,1H), 7.52(t, *J*=8 Hz, 1H), 7.68(m, 2H), 7.89(t, *J*=8 Hz, 1H), 8.02(d, *J*=8.8 Hz, 2H), 8.43(t, *J*=8.8 Hz, 2H), 8.52(d, *J*=8.8 Hz, 1H), 8.73(d, *J*=8.8 Hz, 1H); EI-MS (70 eV) *m/z*(%) 388(M<sup>+</sup>, 100), 325(30), 194(15), 148(17), 106(8), 77(6).

Complex C<sub>5</sub>: orange solid, 75% yield; m.p. 270.8-271.6 °C; <sup>1</sup>H NMR(400 MHz, CDCl<sub>3</sub>) δ 7.30(s, 1H), 7.64(d, *J*=8 Hz, 2H), 7.69(t, *J*=8 Hz, 1H), 7.80(q, *J*=8 Hz, 2H), 8.02(t, *J*=8 Hz, 1H), 8.09(d, *J*=8Hz, 2H), 8.52(d, *J*=8 Hz, 2H), 8.62(d, *J*=8 Hz, 1H), 8.84(d, *J*=8 Hz, 1H); EI-MS (70 eV) *m/z*(%) 370(M<sup>+</sup>, 100), 305(47), 102(11).

### General procedure for the synthesis of Complex C<sub>6</sub>



#### (1) Synthetic procedure for precursor P<sub>1</sub>

At room temperature and nitrogen flow, the mixture of 2-bromo-6-methylphenanthridine (11 mmol) and [4-(1,2,2-triphenylvinyl)phenyl]boronic acid (10 mmol) in dioxane/H<sub>2</sub>O (4:1, V/V, 20 mL) were injected into the mixture of Pd(PPh<sub>3</sub>)<sub>4</sub> (0.5 mmol) and K<sub>2</sub>CO<sub>3</sub> (12 mmol) in dioxane/H<sub>2</sub>O (4:1, V/V, 5 mL). The resulted suspension was heated at 80°C and stirred for 12h. After cooling to the room temperature, the mixture was filtrated. The filtrate was diluted with water (50 mL) and extracted with ethyl acetate (10×3 mL). The combined organic layers were dried over anhydrous Na<sub>2</sub>SO<sub>4</sub> and then evaporated under the reduced pressure. The residue was purified on a silica-gel column chromatography with petroleum ether/CH<sub>2</sub>Cl<sub>2</sub> (3:1) as the eluent.

White solid, 88% yield; m.p. 207.5-208.7°C; <sup>1</sup>H NMR(400 MHz, CDCl<sub>3</sub>) δ 3.06(s, 3H), 7.06-7.19(m, 17H), 7.54(d, *J*=8 Hz, 2H), 7.71(t, *J*=8 Hz, 1H), 7.84(t, *J*=8 Hz, 1H), 7.90(dd, *J*<sub>1</sub>=8.8 Hz, *J*<sub>2</sub>=1.6 Hz, 1H), 8.11(d, *J*=8.8 Hz, 1H), 8.22(d, *J*=8 Hz, 1H), 8.67(m, 2H); <sup>13</sup>C NMR(100 MHz, CDCl<sub>3</sub>) δ 23.99, 119.96, 122.37, 123.90, 126.14, 126.48, 126.55, 126.58, 126.63, 126.65, 127.67, 127.75, 127.80, 127.84, 129.66, 130.44, 131.37, 131.38, 131.45, 131.99, 132.65, 138.64, 138.69, 140.48, 141.34, 143.14, 143.73, 143.75, 143.76, 158.76; EI-MS (70 eV) *m/z*(%) 523(M<sup>+</sup>, 100), 446(10), 253(18), 222(10), 165(11).

#### (2) Synthetic procedure for ligand L<sub>6</sub>

At room temperature and nitrogen atmosphere, 6-methyl-2-[4-(1,2,2-triphenylvinyl)phenyl]phenanthridine (10 mmol) in dried THF (20 mL) was added drop wise to a solution of *n*-BuLi (15 mmol) in dried THF (20 mL). After the solution was stirred for 30 min, ethyl benzoate (10 mmol) in dried THF (20 mL) was added drop wise to the above solution. The mixture was heated at 45 °C for 24h and the precipitate was collected by filtration. After

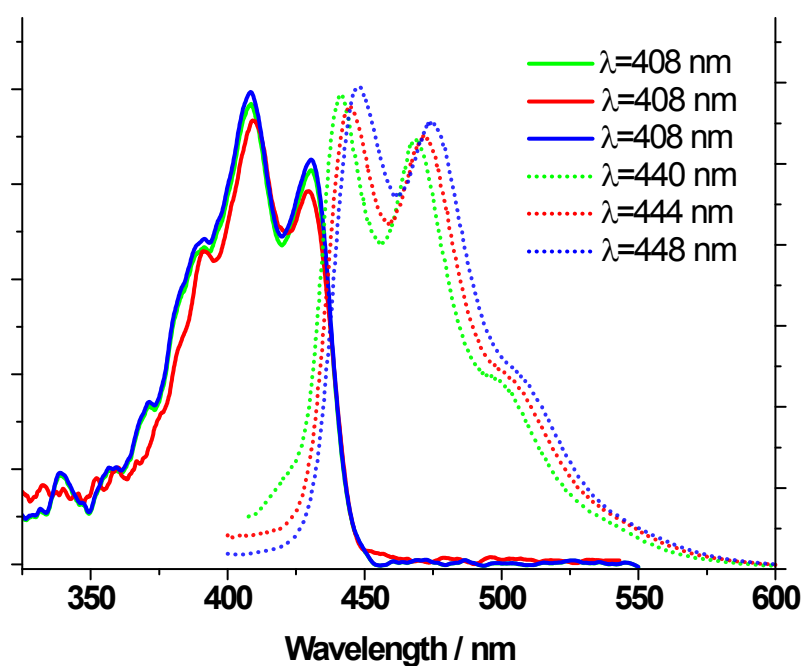
washed with dried THF for 2-3 times, the solid was dissolved in 1% HCl aqueous solution. The solution was extracted by ether (3×10 mL) and the combined organic layer was dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>. After removal of solvent, the residue was purified on a silica-gel column chromatography with ethyl acetate/hexane (6:1) as eluent. Orange solid, 54% yield; m.p. 254.1-256.4°C; <sup>1</sup>H NMR(400 MHz, CDCl<sub>3</sub>) δ 6.84(s, 1H), 7.05-7.15(m, 17H), 7.44(d, *J*=8.0 Hz, 2H), 7.49(d, *J*=6.3 Hz, 4H), 7.61(t, *J*=7.6 Hz, 1H), 7.71(d, *J*=8.1 Hz, 1H), 7.78(t, *J*=7.6 Hz, 1H), 8.05(d, *J*=3.6 Hz, 2H), 8.28(d, *J*=8.2, Hz, 1H), 8.36(s, 1H), 8.42(d, *J*=8.2 Hz, 1H), 15.95(s, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 85.43, 118.42, 120.40, 120.44, 122.60, 124.41, 125.16, 126.06, 126.46, 126.52, 126.55, 126.89, 127.63, 127.71, 127.81, 128.11, 128.34, 128.74, 130.66, 131.32, 131.34, 131.40, 131.94, 131.96, 132.05, 133.86, 135.96, 138.07, 140.36, 140.62, 141.23, 142.94, 143.65, 143.68, 143.70, 152.42, 186.85; EI-MS (70 eV) *m/z*(%) 628(M<sup>+</sup> +1, 100), 607(21), 570(15), 457(17), 371(23), 327(23), 284(38), 256(27), 239(17), 194(20), 177(12), 133(19).

### (3) Synthetic procedure for complex C<sub>6</sub>

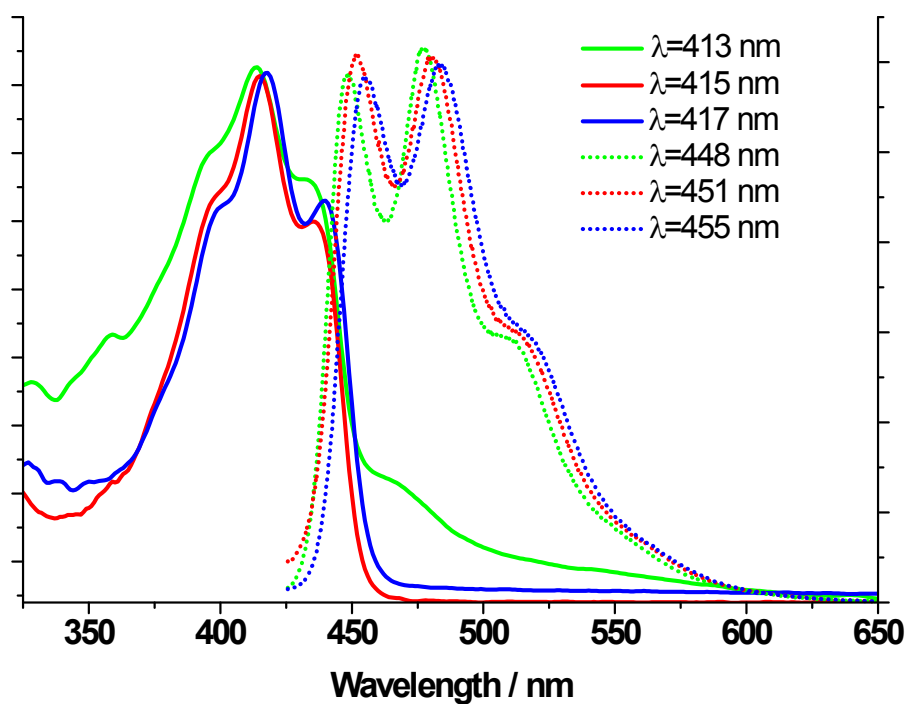
At room temperature, triethylamine (3 mmol) in dried CH<sub>2</sub>Cl<sub>2</sub> (1 mL) was added drop wise to a solution of (Z)-1-phenyl-2-(2-(4-(1,2,2-triphenylvinyl)phenyl)phenanthridin-6(5H)-ylidene)ethanone (1 mmol) in dried CH<sub>2</sub>Cl<sub>2</sub> (2 mL). After the solution was stirred for 30 min, boron trifluoride etherate (8 mmol) in dried CH<sub>2</sub>Cl<sub>2</sub> (2 mL) was added drop wise. The mixture was stirred overnight and the solvent was removed on a rotating evaporator. The residue was purified by a flash column chromatography on silica gel with dried CH<sub>2</sub>Cl<sub>2</sub> as eluent. Yellow solid, 67% yield; m.p. 325.7-327.3°C; <sup>1</sup>H NMR(400 MHz, CDCl<sub>3</sub>) δ 7.07-7.20(m, 17H), 7.52(m, 5H), 7.78(t, *J*=7.6 Hz, 1H), 7.92(d, *J*=8.8 Hz, 1H), 7.97(d, *J*=8 Hz, 1H), 8.13(d, *J*= 7.2 Hz, 2H), 8.51(d, *J*=8.4 Hz, 1H), 8.61(s, 1H), 8.66(d, *J*=8 Hz, 1H), 8.83(d, *J*=8.8 Hz, 1H); EI-MS (70 eV) *m/z*(%) 676(M<sup>+</sup> +1, 52), 663(40), 628(100), 610(30), 568(22), 536(20), 503(18), 355(24), 284(96), 256(55), 239(20), 133(21).

## References

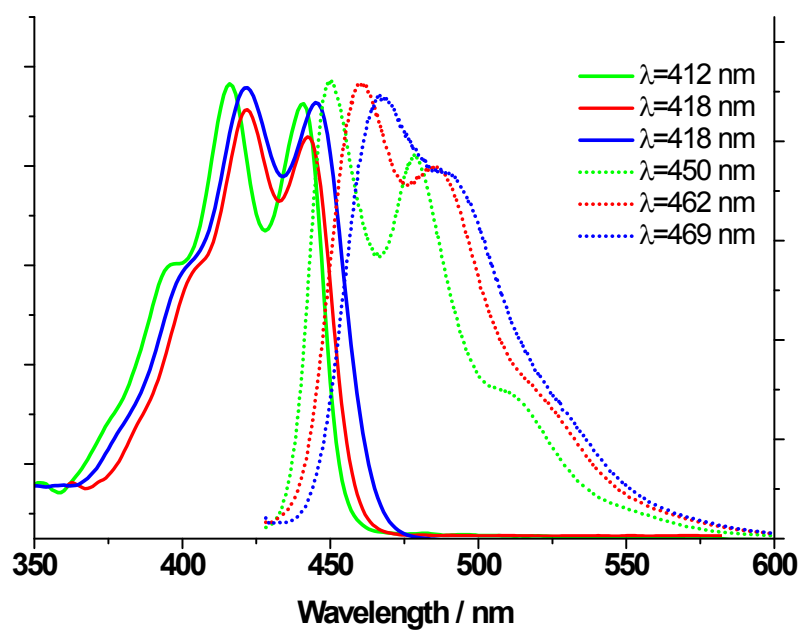
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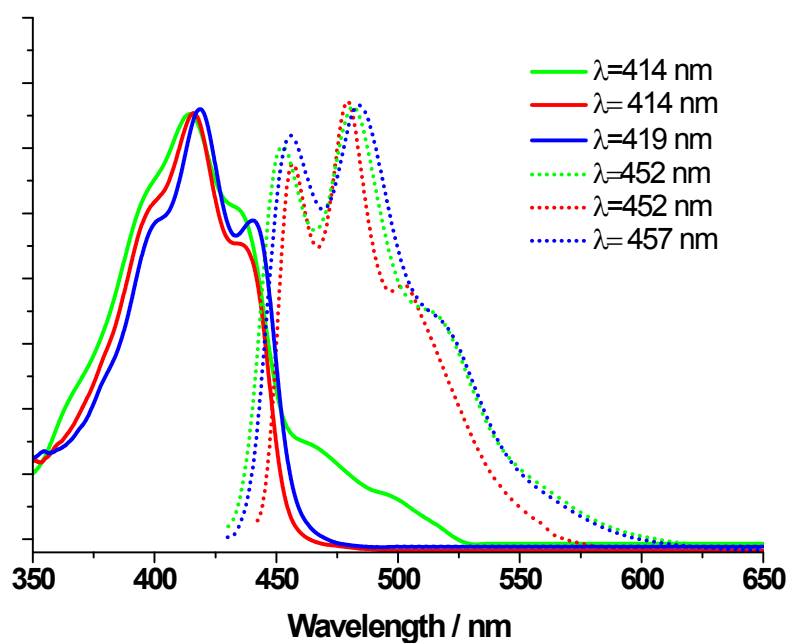
**Fig. S1** Normalized absorption (solid line) and emission spectra (dot line) of C<sub>1</sub> in different solvents (green: hexane; red: CH<sub>2</sub>Cl<sub>2</sub>; blue: DMSO)



**Fig. S2** Normalized absorption (solid line) and emission spectra (dot line) of C<sub>2</sub> in different solvents (green: hexane; red: CH<sub>2</sub>Cl<sub>2</sub>; blue: DMSO)



**Fig. S3** Normalized absorption (solid line) and emission spectra (dot line) of C<sub>3</sub> in different solvents (*green*: hexane; *red*: CH<sub>2</sub>Cl<sub>2</sub>; *blue*: DMSO)



**Fig. S4** Normalized absorption (solid line) and emission spectra (dot line) of C<sub>5</sub> in different solvents (*green*: hexane; *red*: CH<sub>2</sub>Cl<sub>2</sub>; *blue*: DMSO)



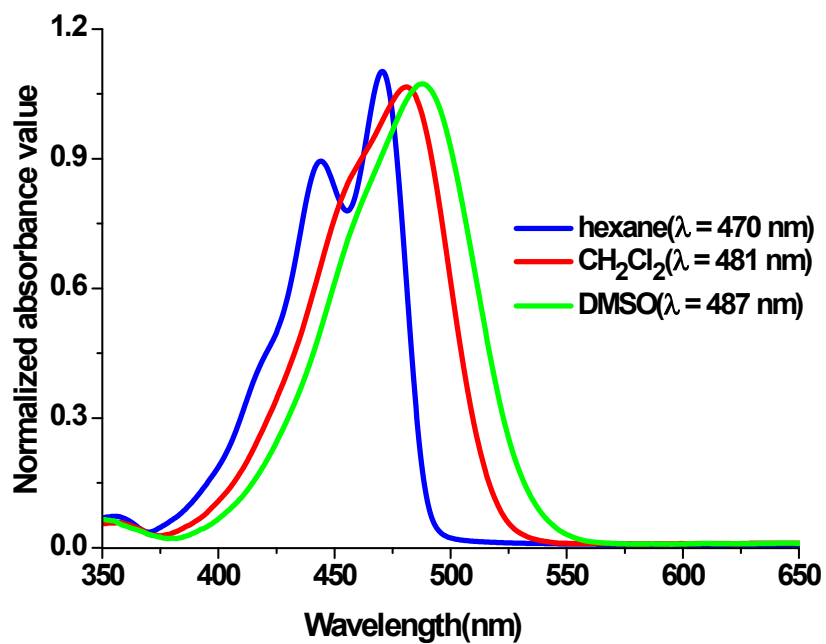


Fig. S5 Normalized absorption spectra of C<sub>4</sub> in different solvents

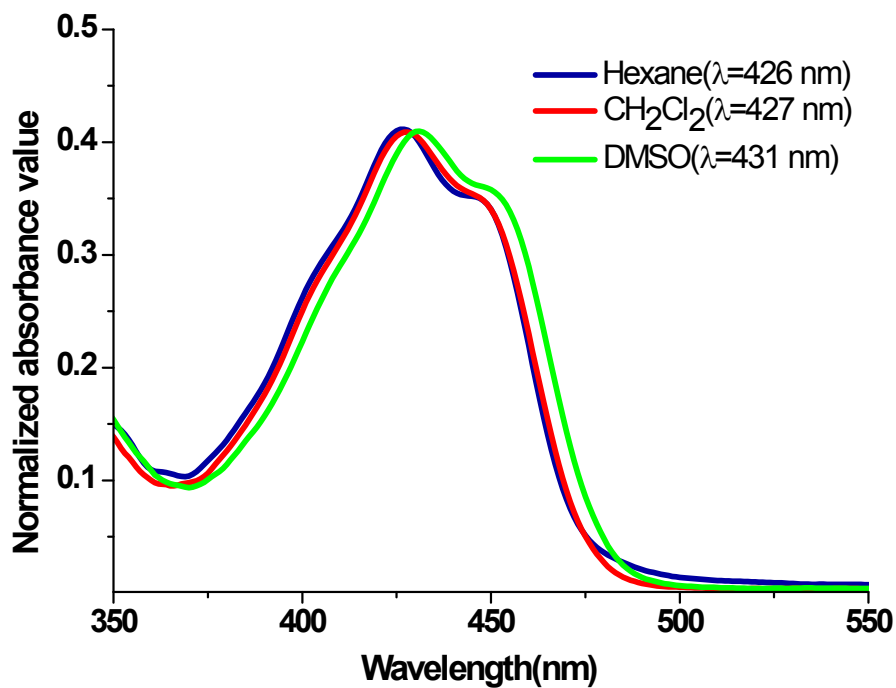


Fig. S6 Normalized absorption spectra of C<sub>6</sub> in different solvents

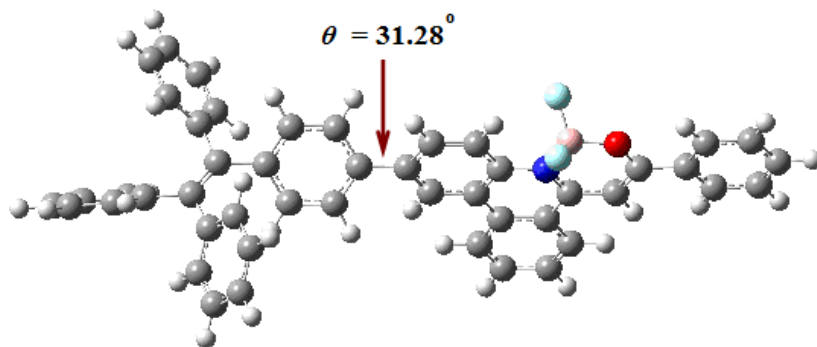


Fig. S7 The simulated geometry of C<sub>6</sub>

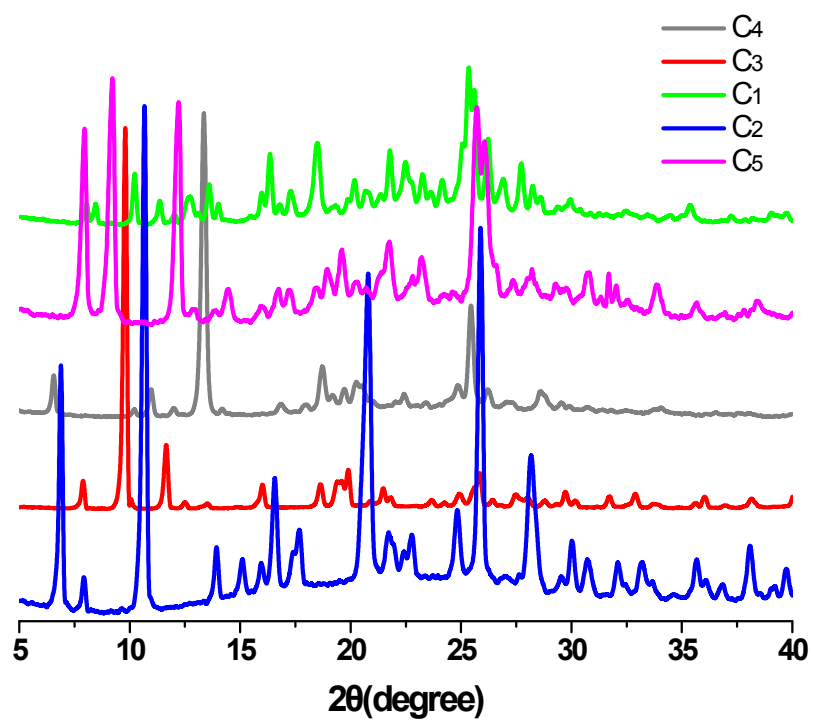


Fig. S8 Powder XRD diagrams of C<sub>1</sub>-C<sub>5</sub> solids

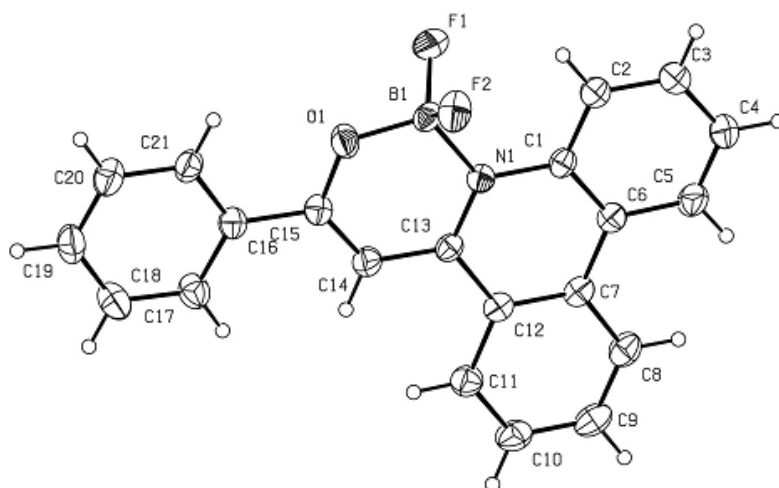


Fig. S9 ORTEP drawing of  $C_1$  molecule

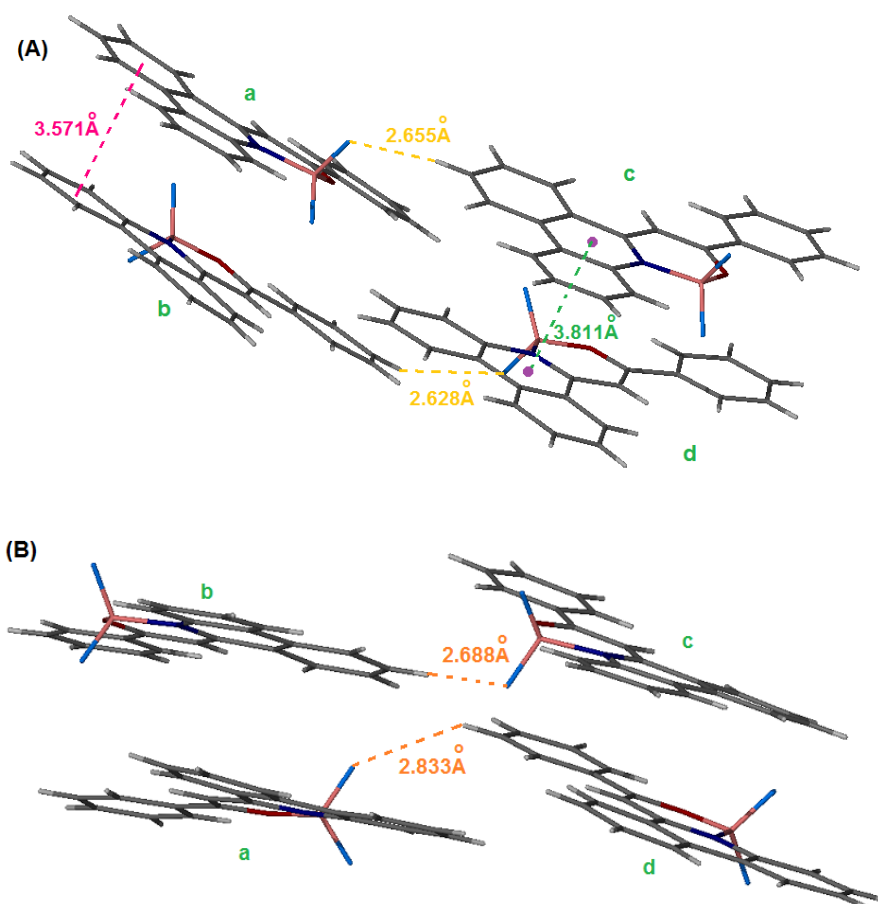


Fig. S10  $\pi$ - $\pi$  and C-H $\cdots$ F interactions in different molecule pairs of  $C_1$

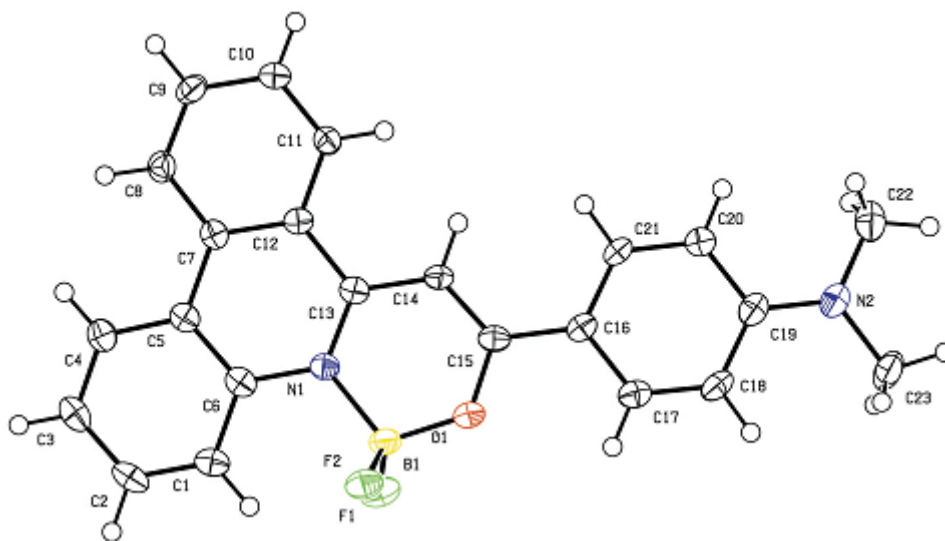


Fig. S11 ORTEP drawing of C<sub>4</sub> molecule

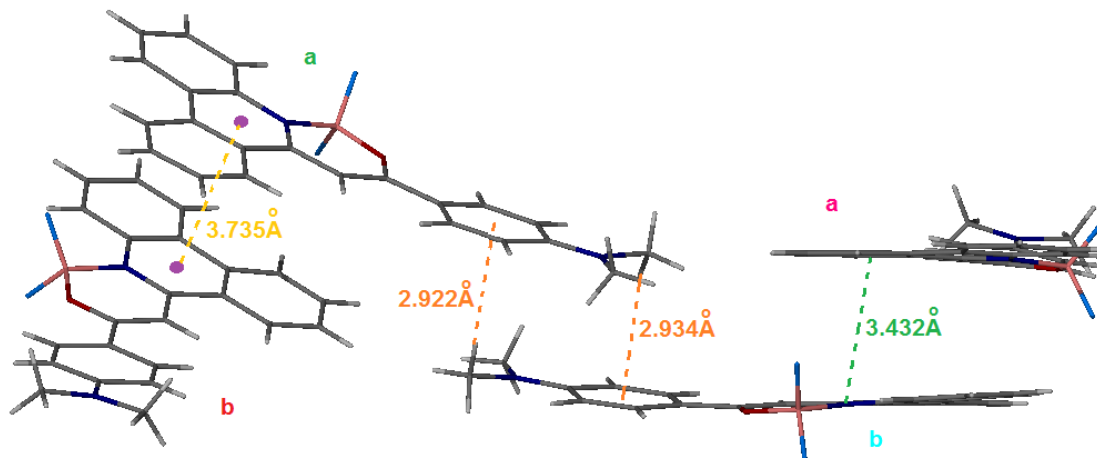
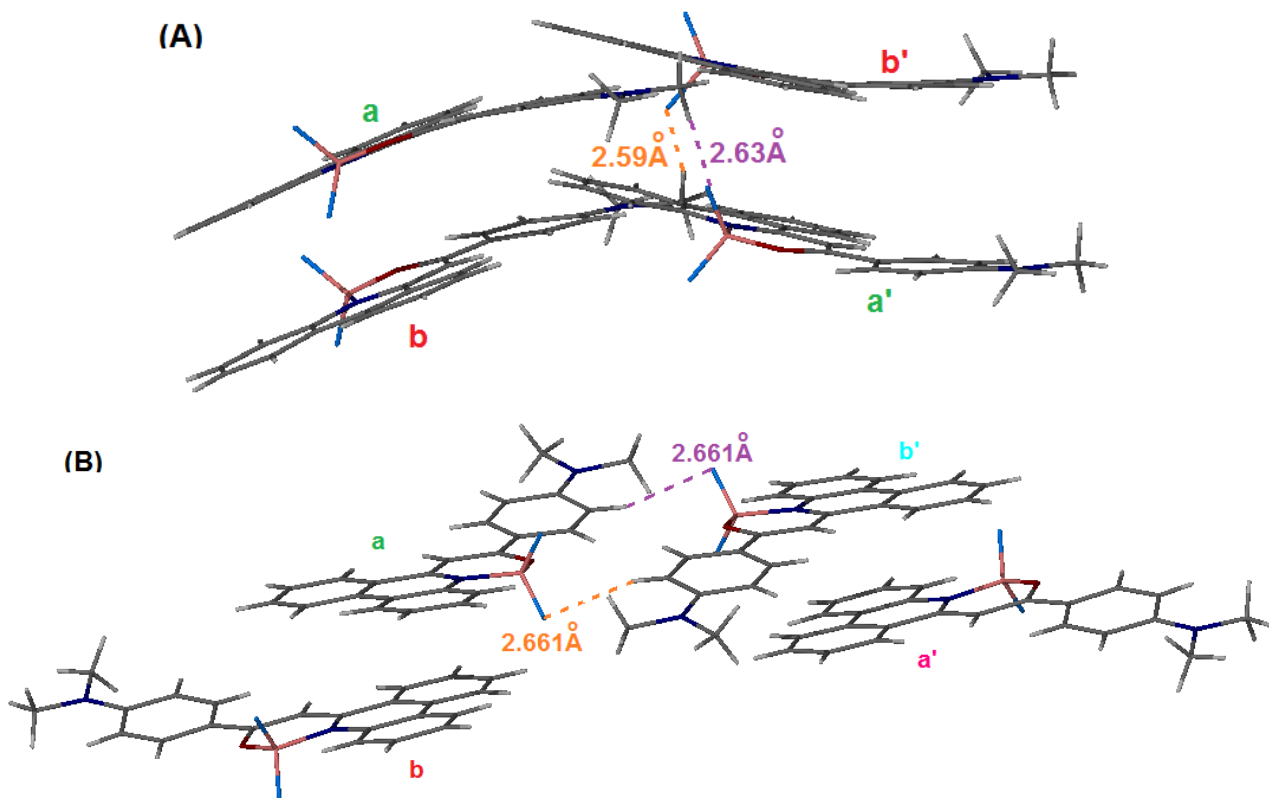
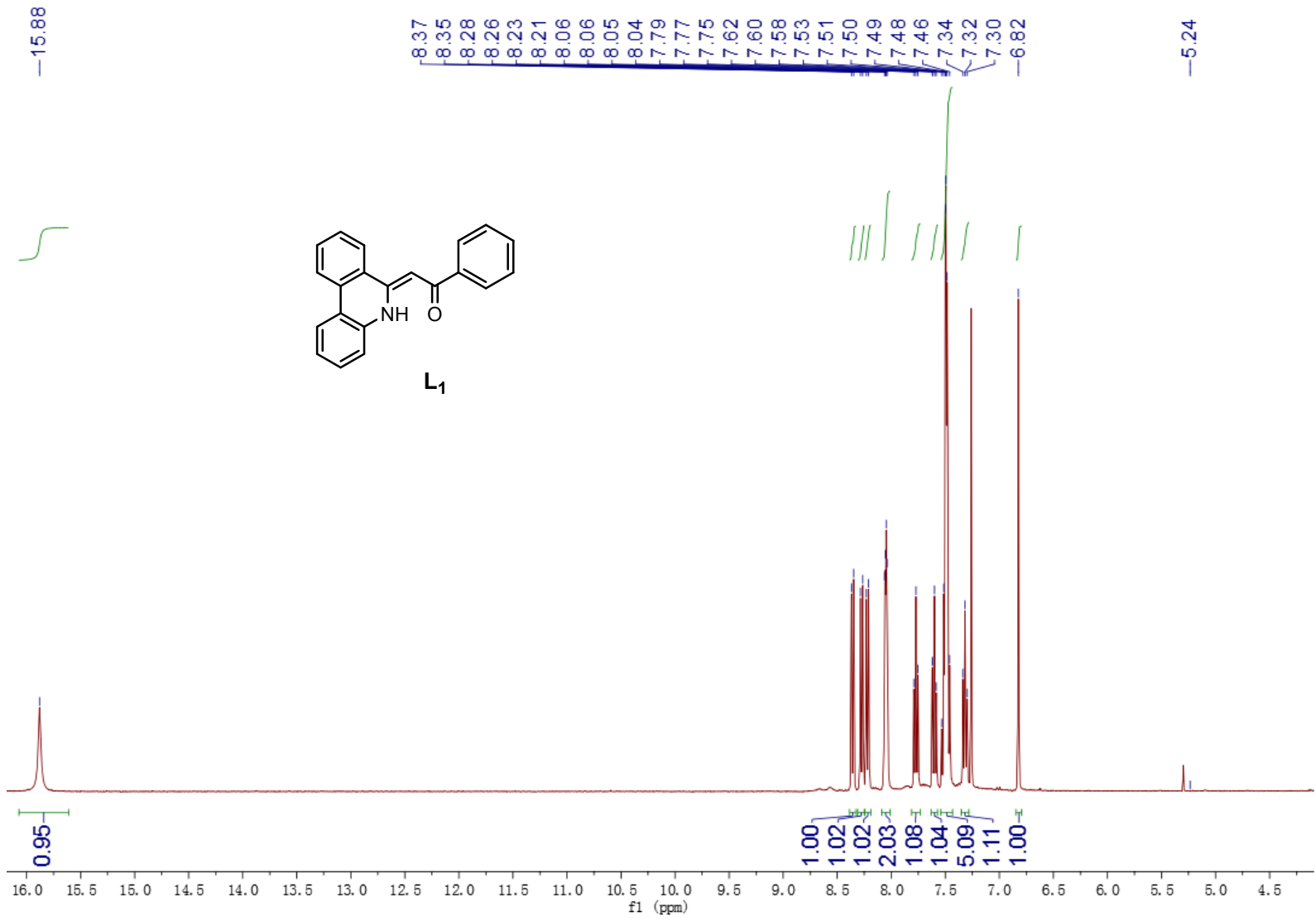
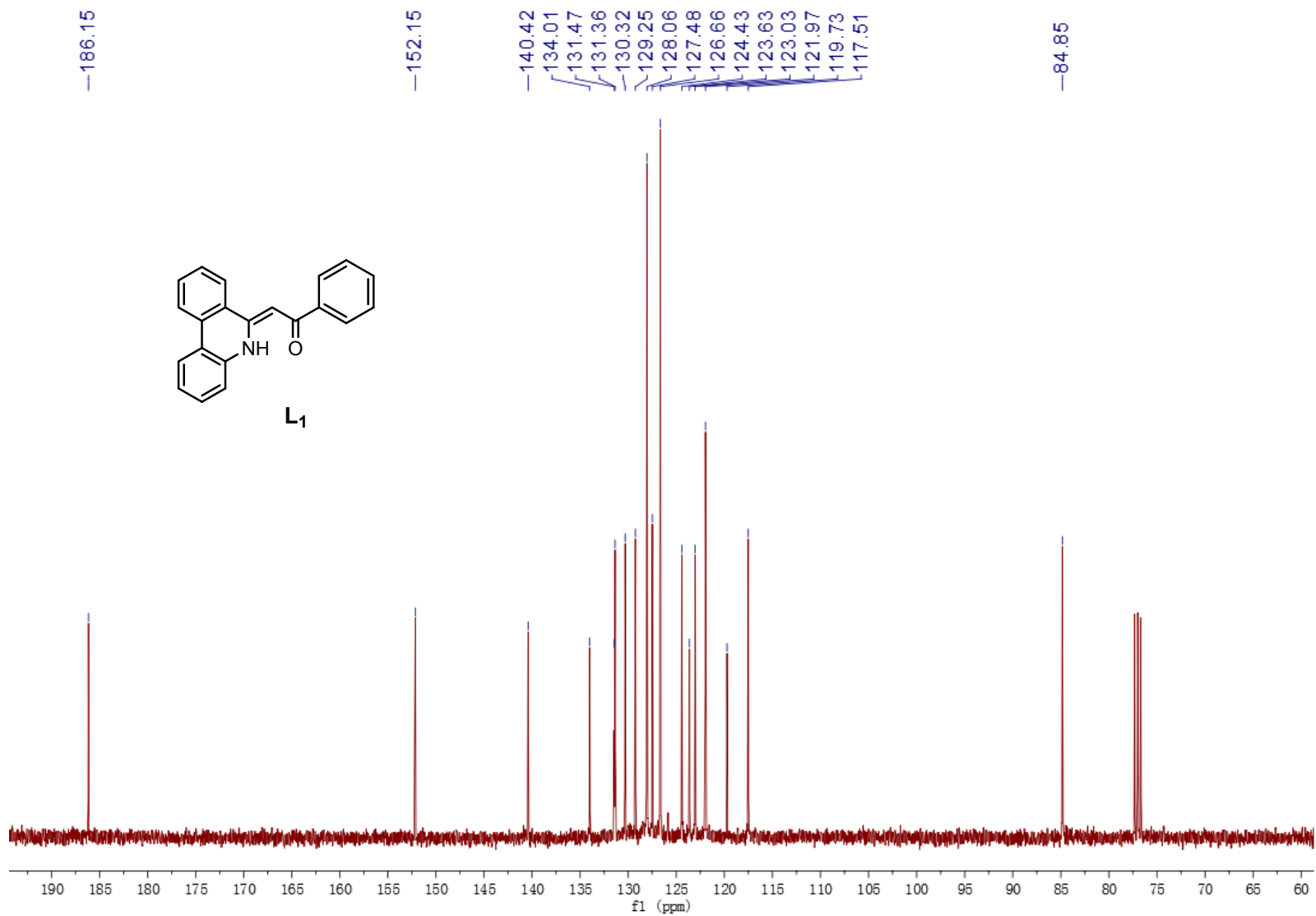
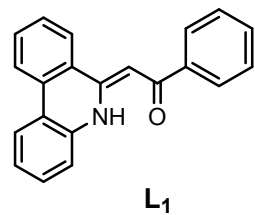
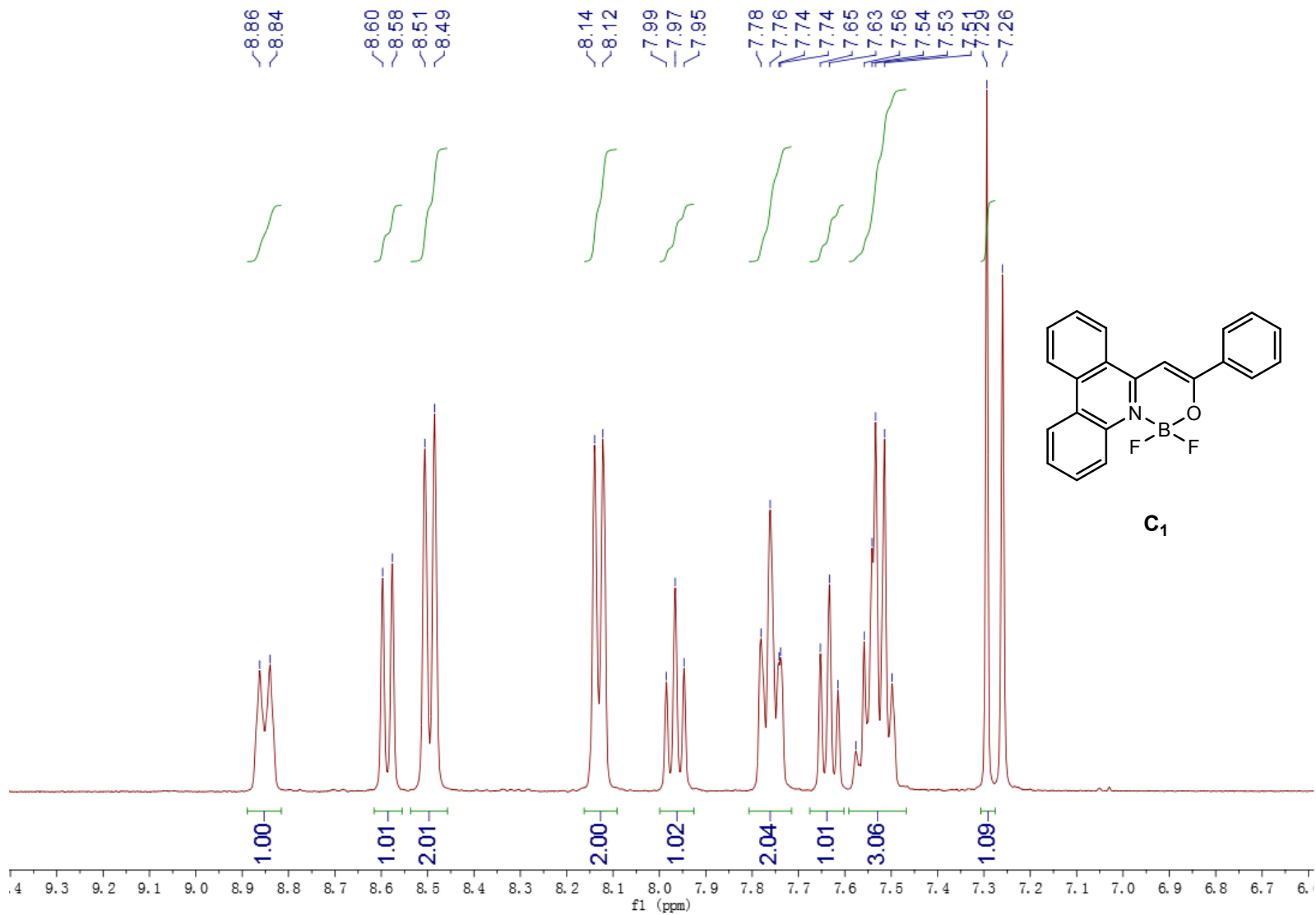


Fig. S12  $\pi$ - $\pi$  and C-H $\cdots$  $\pi$  interactions among C<sub>4</sub> molecules

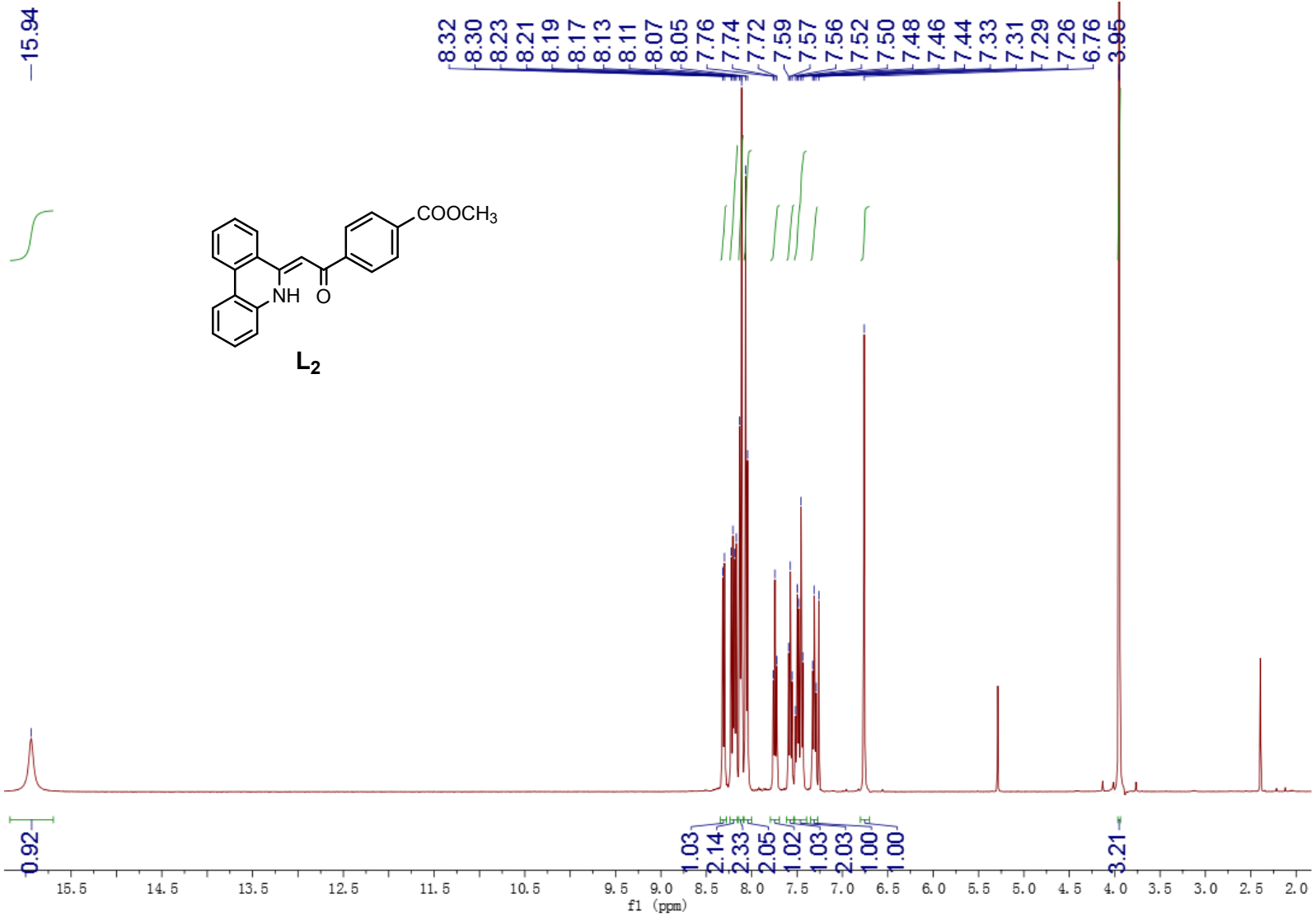


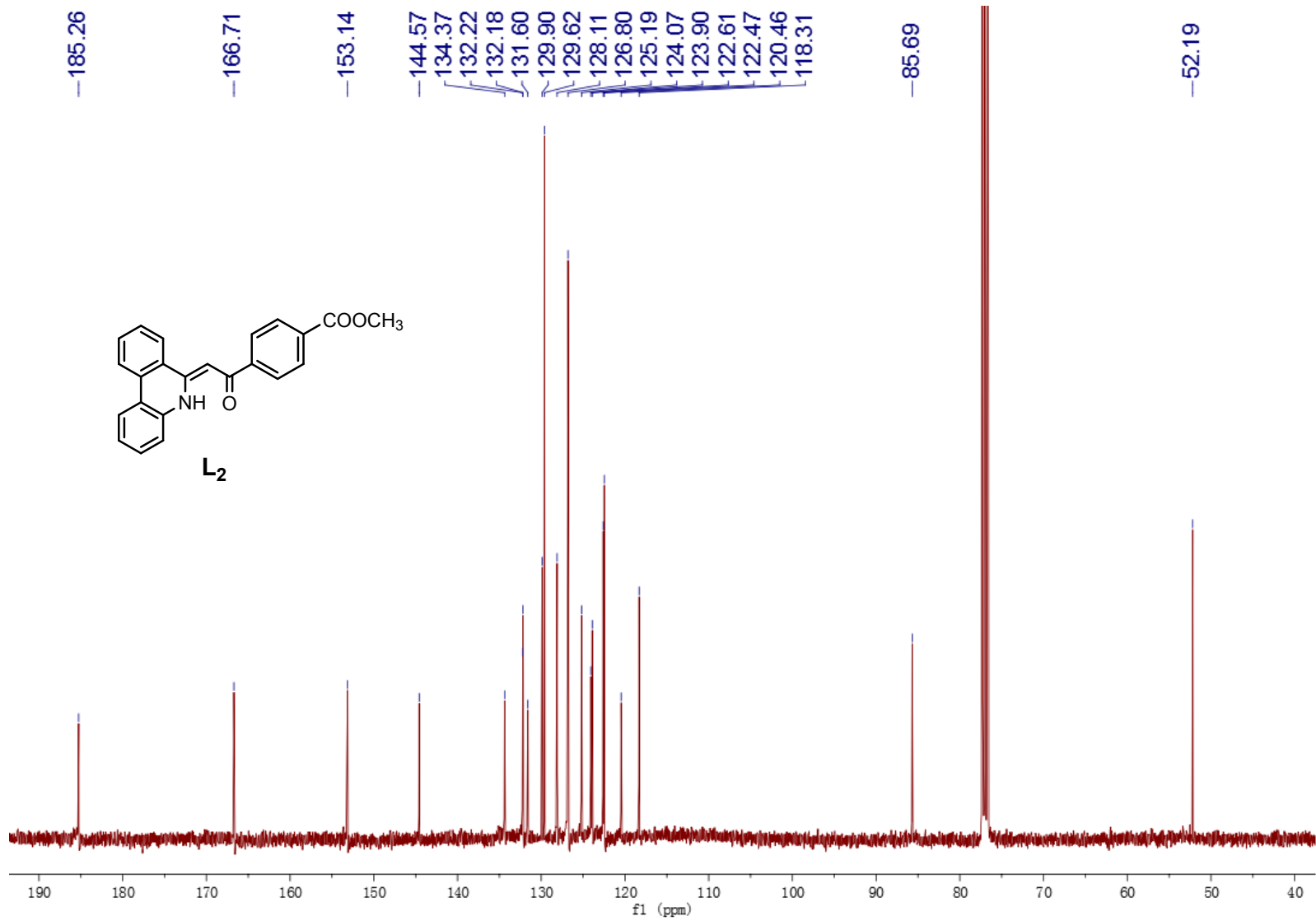


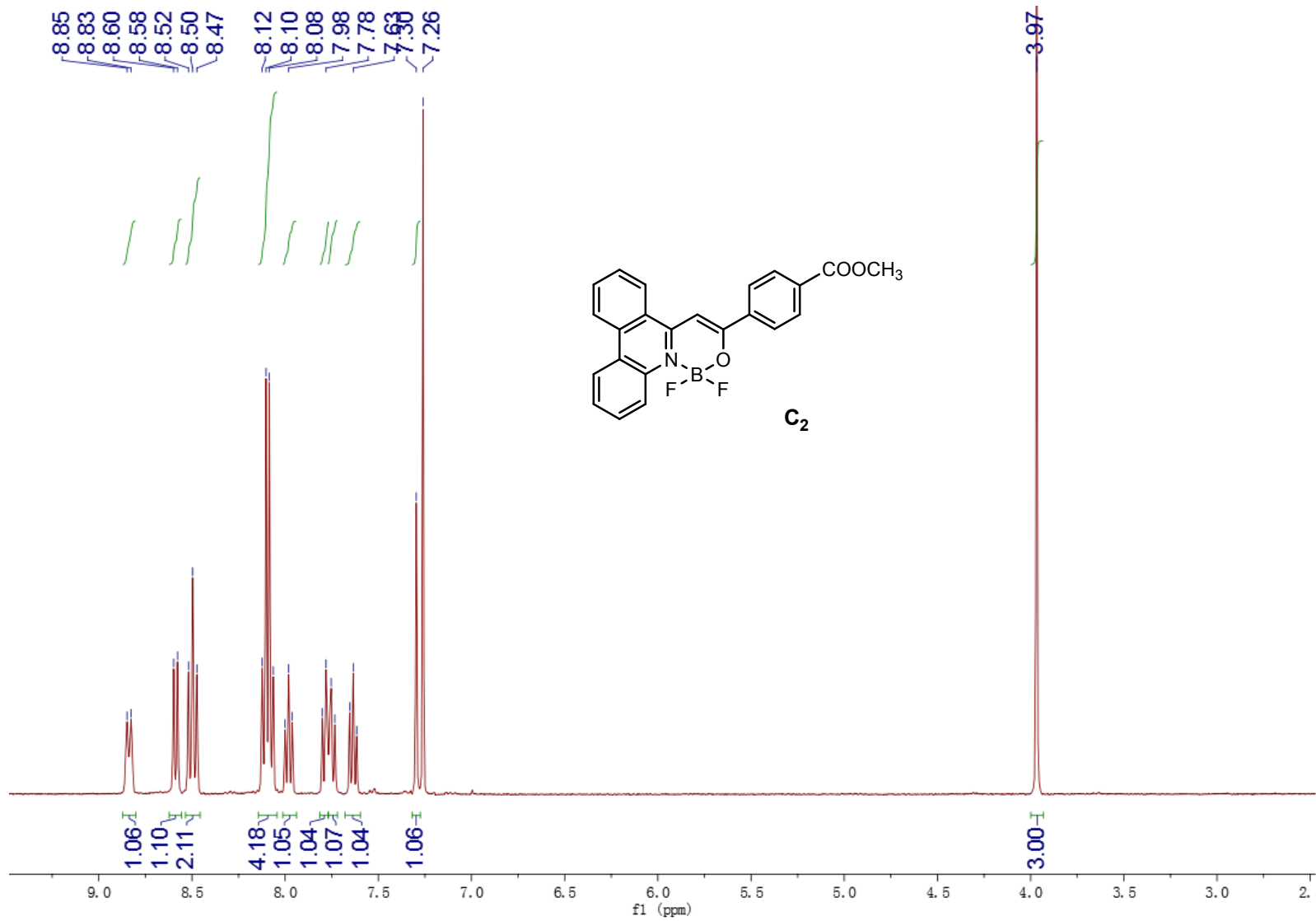


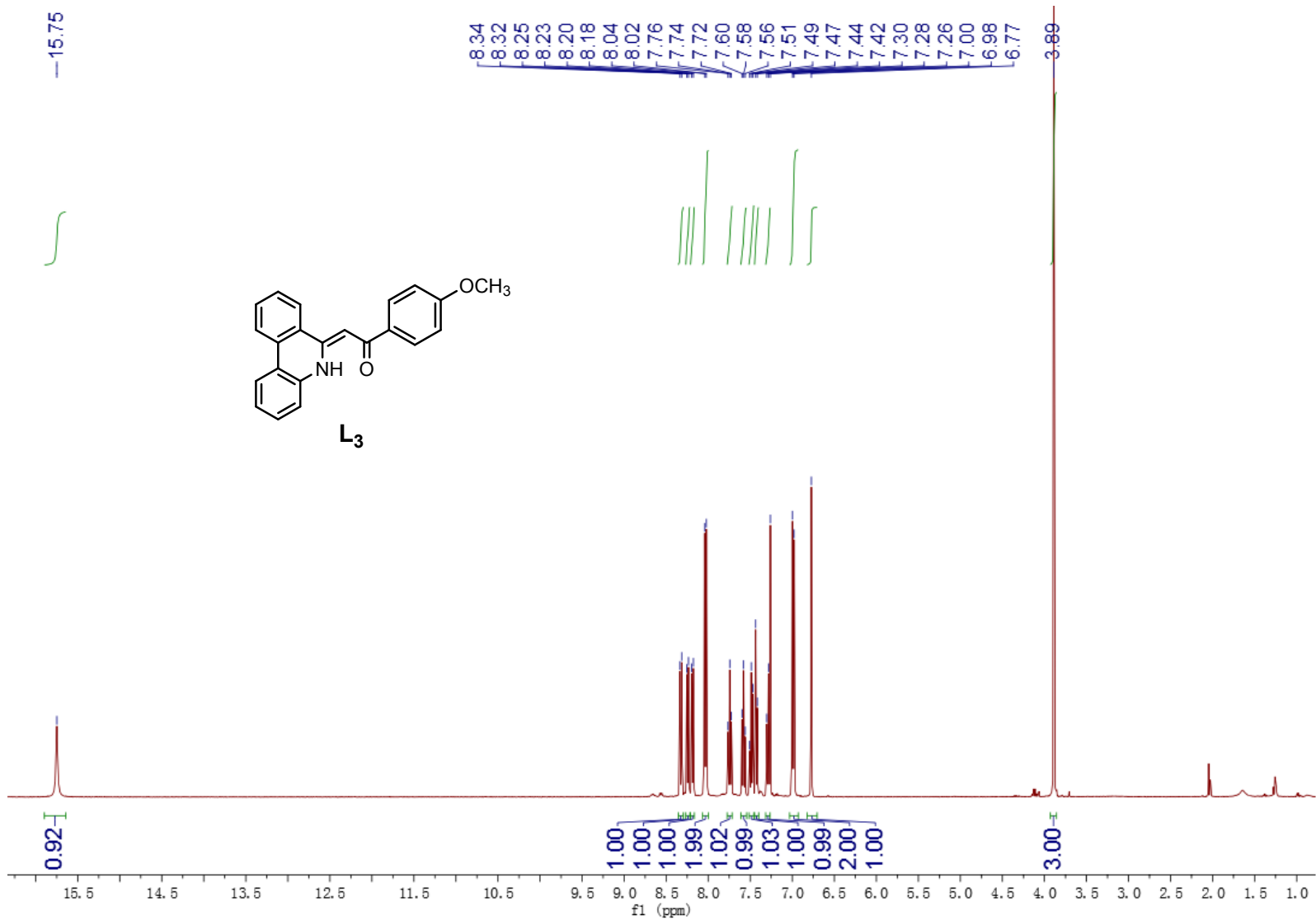












5-C

