Supplementary Materials

for

Unsymmetrical Hexafluorocyclopentene-linked Twist π-Conjugated Molecules as Dual-State Emissive Luminophores

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1. Synthesis

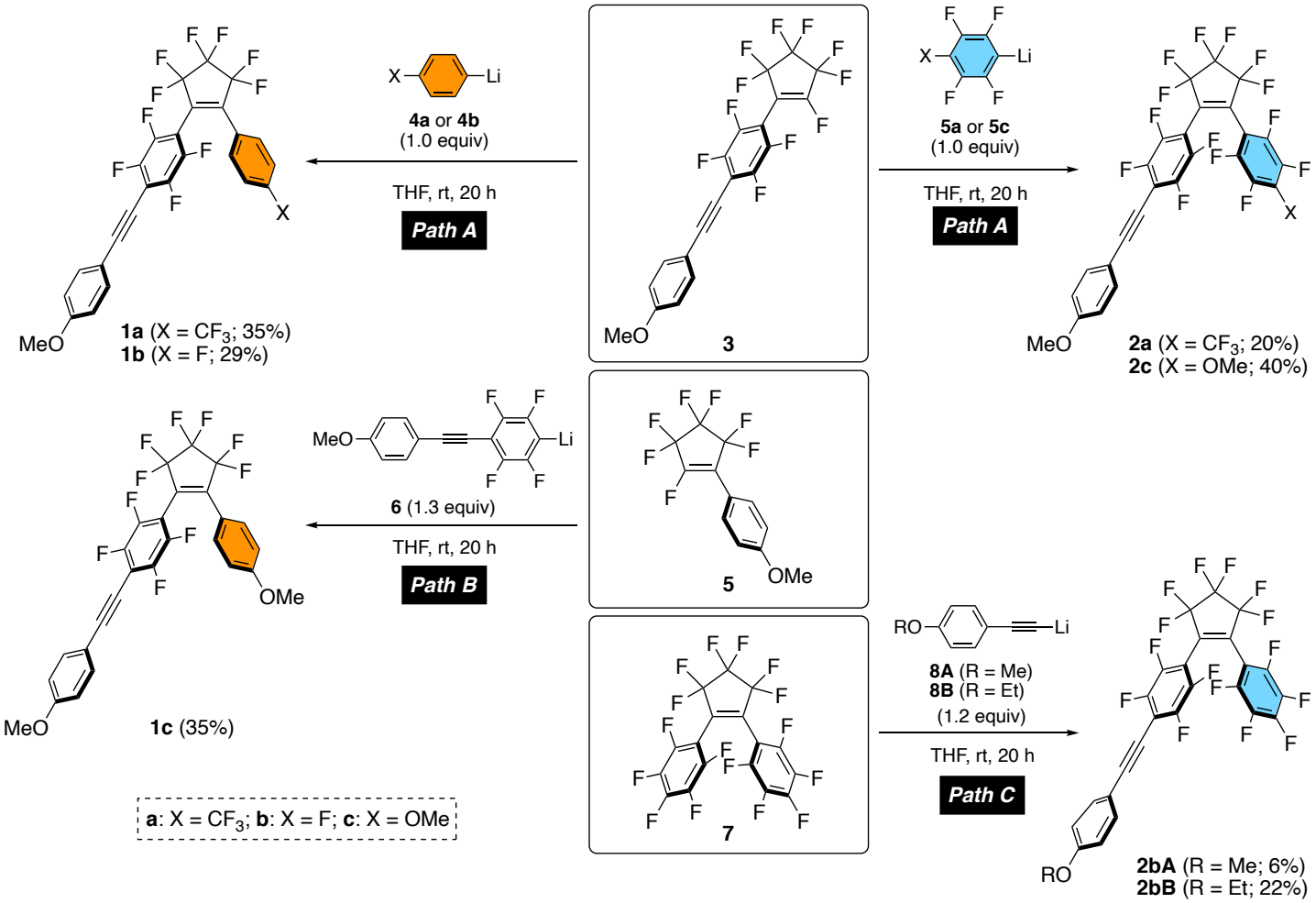


Figure S1. Synthetic scheme for the unsymmetrical twist p-conjugated molecules **1a**–**c** and **2a**–**c** used in this study.

1.1. Typical procedure for the synthesis of 1-[2,3,5,6-Tetrafluoro-4-{2(4-methoxyphenyl)ethyn-1-yl}phenyl]-2-(4-trifluoromethylphenyl)-3,3,4,4,5,5-hexafluorocyclopentene (1a): Path A

In a two-necked round-bottomed flask, equipped with a Teflon®-coated stirrer bar, was placed 4-bromobenzotrifluoride (0.122 g, 0.5 mmol) in THF (2.0 mL). To the solution was added slowly *n*-BuLi (1.6 mol L^{-1} hexane solution, 0.36 mL, 0.6 mmol) and the reaction mixture was stirred at that temperature for 0.5 h. To the resultant was added 1-[2,3,5,6-Tetrafluoro-4-{2(4-methoxyphenyl)ethyn-1-yl}phenyl]-2,3,3,4,4,5,5-heptafluorocyclopentene (**3**, 0.38 g, 0.55 mmol) in THF (5 mL) at –78 °C and the whole was raised up to 25 °C and continuously stirred at the temperature for 20 h. The resultant was poured into saturated aqueous NH_4Cl solution (20 mL), and the crude product was extracted with Et_2O (10 mL, three times) and organic layer was washed with brine (20 mL, once). Organic layer collected was dried over anhydrous Na_2SO_4, which was separated by atmospheric filtration. The filtrate was evaporated in vacuo and subjected to silica-gel column chromatography (eluent: hexane/EtOAc = 10/1), followed by recrystallization from CH_2Cl_2/MeOH (v/v = 1/1), to obtain the title compound **1a** in 35% yield (0.10 g, 0.2 mmol) as a white solid.

*1.1.1. 1-[2,3,5,6-Tetrafluoro-4-{2(4-methoxyphenyl)ethyn-1-yl}phenyl]-2-(4-trifluoromethylphenyl)-3,3,4,4,5,5-hexafluorocyclopentene (**1a**)*

Yield: 35% (yellow solid); m.p.: 121.6–124.2 °C; ^{1}H NMR ($CDCl_3$): δ 3.85 (s, 3H), 6.91 (d, J = 8.8 Hz, 2H), 7.47 (d, J = 8.4 Hz, 2H), 7.52 (d, J = 8.8 Hz, 2H), 7.68 (d, J = 8.4 Hz, 2H); ^{13}C NMR ($CDCl_3$): δ 55.4, 72.8 (t, J = 4.4 Hz), 104.9

(t, *J* = 3.7 Hz), 105.9 (t, *J* = 19.1 Hz), 108.5 (t, *J* = 17.6 Hz), 110.8 (t, *J* = 24.9 Hz), 112.0–119.0 (m, 3F), 113.1, 114.3, 123.3 (q, *J* = 272.2 Hz), 126.2 (q, *J* = 3.7 Hz), 128.6, 130.0, 133.3 (q, *J* = 33.7 Hz), 133.8, 143.9 (dd, *J* = 252.3, 14.7 Hz), 146.5 (tt, *J* = 23.4, 6.6 Hz), 146.6 (dd, *J* = 254.5, 13.9 Hz), 161.1; ^{19}F NMR ($CDCl_3$): δ –63.80 (s, 3F), –111.4 (s, 2F), –111.8 (brs, 2F), –132.28 (t, *J* = 4.1 Hz, 2F), –135.02 to –135.17 (m, 2F), –138.65 to –138.84 (m, 2F); IR (KBr): ν 2979, 22851, 2224, 1603, 1478, 1324, 1134, 980, 839 cm^{-1}; HRMS: (FAB+) *m/z* $[M]^+$ calcd for $C_{27}H_{11}F_{13}O$: 598.0602; found: 598.0602.

*1.1.2. 1-[2,3,5,6-Tetrafluoro-4-{2(4-methoxyphenyl)ethyn-1-yl}phenyl]-2-(4-fluorophenyl)-3,3,4,4,5,5-hexafluorocyclopentene (**1b**)*

Yield: 29% (white solid); m.p.: 101.4–101.9 °C; ^{1}H NMR ($CDCl_3$): δ 3.85 (s, 3H), 6.92 (d, *J* = 8.8 Hz, 2H), 7.10 (t, *J* = 8.8 Hz, 2H), 7.35 (dd, *J* = 8.8, 4.8 Hz, 2H), 7.53 (d, *J* = 8.8 Hz, 2H); ^{13}C NMR ($CDCl_3$): δ 55.4, 72.9 (t, *J* = 3.6 Hz), 104.7 (t, *J* = 3.6 Hz), 106.6 (t, *J* = 19.1 Hz), 108.2 (t, *J* = 15.3 Hz), 110.8 (t, *J* = 24.8 Hz), 112.0–119.1 (m), 113.2, 114.3, 116.7 (d, *J* = 22.7 Hz), 122.6 (d, *J* = 2.2 Hz), 127.6 (t, *J* = 23.5 Hz), 130.4 (d, *J* = 8.8 Hz), 133.7, 143.9 (dd, *J* = 251.5, 13.9 Hz), 146.57 (t, *J* = 24.2 Hz), 146.6 (dd, *J* = 254.4, 13.9 Hz), 161.0, 163.1, 165.6; ^{19}F NMR ($CDCl_3$): δ –107.01 to –107.13 (m, 1F), –111.48 (s, 2F), –111.59 (s, 2F), –132.40 (quin, *J* = 5.3 Hz, 2F), –135.37 (q, *J* = 9.4 Hz, 2F), –138.69 to –138.90 (m, 2F); IR (KBr): ν 3028, 2948, 2850, 2209, 1603, 1515, 1486, 1251, 1139, 1058, 981, 831 cm^{-1}; HRMS: (FAB+) *m/z* $[M]^+$ calcd for $C_{26}H_{11}F_{11}O$: 548.0634; found: 548.0628.

*1.1.3. 1-[2,3,5,6-Tetrafluoro-4-{2(4-methoxyphenyl)ethyn-1-yl}phenyl]-2-{4-(trifluoromethyl)-2,3,5,6-tetrafluorophenyl}-3,3,4,4,5,5-hexafluorocyclopentene (**2a**)*

Yield: 20% (white solid); m.p.: 142.3–143.2 °C; ^{1}H NMR ($CDCl_3$): δ 3.85 (s, 3H), 6.91 (d, *J* = 8.8 Hz, 2H), 7.52 (d, *J* = 8.8 Hz, 2H); ^{13}C NMR ($CDCl_3$): δ 55.4, 72.8 (t, *J* = 3.6 Hz), 104.2 (t, *J* = 16.9 Hz), 105.8 (t, *J* = 3.6 Hz), 109.5 (t, *J* = 17.6 Hz), 110.2 (t, *J* = 17.6 Hz), 112.9, 114.3, 116.8–118.0 (m), 120.1 (q, *J* = 276.5 Hz), 133.8, 135.5 (t, *J* = 33.7 Hz), 138.0 (t, *J* = 5.8 Hz), 143.6 (dd, *J* = 253.7, 14.7 Hz), 144.1 (dd, *J* = 243.5, 14.7 Hz), 146.7 (dd, *J* = 228.9, 13.2 Hz), 161.2, several carbon signals cannot be assigned due to extremely complex spin-spin coupling between carbon and fluorine atoms; ^{19}F NMR ($CDCl_3$): δ –57.10 (t, *J* = 21.8 Hz, 3F), –111.60 (s, 2F), –111.83 (s, 2F), –132.5 (s, 2F), –134.38 to –134.60 (m, 2F), –135.04 to –135.28 (m, 2F), –137.10 to –137.44 (m, 2F), –138.50 to –138.64 (m, 2F); IR (KBr): ν 3029, 2966, 2851, 2225, 1605, 1485, 1342, 1249, 1159, 1034, 993, 973, 834 cm^{-1}; HRMS: (FAB+) *m/z* $[M]^+$ calcd for $C_{27}H_7F_{17}O$: 670.0225; found: 670.0236.

*1.1.4. 1-[2,3,5,6-Tetrafluoro-4-{2(4-methoxyphenyl)ethyn-1-yl}phenyl]-2-(2,3,5,6-tetrafluoro-4-methoxyphenyl)-3,3,4,4,5,5-hexafluorocyclopentene (**2c**)*

Yield: 40% (white solid); m.p.: 102.9–103.9 °C; ^{1}H NMR ($CDCl_3$): δ 3.85 (s, 3H), 4.16 (s, 3H), 6.91 (d, *J* = 8.8 Hz, 2H), 7.52 (d, *J* = 8.8 Hz, 2H); ^{13}C NMR ($CDCl_3$): δ 55.4, 62.0 (t, *J* = 3.6 Hz), 72.9, 96.8–100.5 (m), 105.0–105.8 (m), 105.1, 108.4–117.8 (m, 3C for $CF_2CF_2CF_2$), 113.1, 114.3, 133.8, 136.0–138.2 (m), 140.7 (dm, *J* = 281.3 Hz), 142.3 (dm, *J* = 202.4 Hz), 144.0 (dm, *J* = 256.3 Hz), 147.0 (dm, *J* = 196.2 Hz), 161.1, several carbon signals cannot be assigned due to extremely complex spin-spin coupling between carbon and fluorine atoms; ^{19}F NMR ($CDCl_3$): δ –111.71 (s, 2F), –111.96(s, 2F), –132.65 (s, 2F), –135.00 (q, *J* = 9.8 Hz, 2F), –138.30 to –138.58 (m, 2F), –138.74 to –138.98 (m, 2F), –155.88 to –156.08 (m, 2F); IR (KBr): ν 3018, 2948, 2845, 2224, 1605, 1494, 1270, 1270, 1166, 1070, 985, 831 cm^{-1}; HRMS: (FAB+) *m/z* $[M]^+$ calcd for $C_{27}H_{10}F_{14}O_2$: 632.0457; found: 632.0449.

1.2. Typical synthetic procedure for 1-[2,3,5,6-Tetrafluoro-4-{2(4-methoxyphenyl)ethyn-1-yl}phenyl]-2-(4-methoxyphenyl)-3,3,4,4,5,5-hexafluorocyclopentene (1c): Path B

In a two-necked round-bottomed flask, equipped with a Teflon®-coated stirrer bar, was placed 1-bromo-2,3,5,6-tetrafluoro-4-{2-(4-methoxyphenyl)ethyn-1-yl}benzene (0.14 g, 0.4 mmol) in THF (4.0 mL) and the solution was cooled to –78 °C. To the solution was added slowly *n*-BuLi (1.6 mol L^{-1} hexane solution, 0.30 mL, 0.5 mmol) and the whole was stirred at –78 °C for 0.5 h. To the resultant solution was added 1-(4-methoxyphenyl)-2,3,3,4,4,5,5-heptafluorocyclopentene (**5**, 0.086 g, 0.29 mmol) in THF (4.0 mL), and the reaction temperature was raised up to 25 °C and the whole was stirred at 25 °C for 12 h. The reaction mixture was poured into saturated aqueous NH4Cl solution (20 mL), and the crude product was extracted with Et_2O (10 mL, three times) and organic layer was washed with brine (20 mL, once). Organic layer collected was dried over anhydrous Na_2SO_4, which was separated by atmospheric filtration. The filtrate was evaporated in vacuo and subjected to silica-gel column chromatography (eluent: hexane/EtOAc = 10/1), followed by recrystallization from CH_2Cl_2/MeOH (v/v = 1/1), to obtain the title compound **1c** in 35% yield (0.076 g, 0.1 mmol) as a white solid.

*1.2.1. 1-[2,3,5,6-Tetrafluoro-4-{2(4-methoxyphenyl)ethyn-1-yl}phenyl]-2-(4-methoxyphenyl)-3,3,4,4,5,5-hexafluorocyclopentene (**1c**)*

Yield: 35% (white solid); m.p.: 111.9–113.1 °C; ^{1}H NMR ($CDCl_3$): δ 3.81 (s, 3H), 3.84 (s, 3H), 6.87 (d, J = 8.9 Hz, 2H), 6.90 (d, J = 8.9 Hz, 2H), 7.29 (d, J = 8.8 Hz, 2H), 7.52 (d, J = 8.8 Hz, 2H); ^{13}C NMR ($CDCl_3$): δ 55.4, 72.9 (t, J = 4.4 Hz), 104.3 (t, J = 3.7 Hz), 107.5 (t, J = 19.1 Hz), 107.8 (tt, J = 17.8, 2.5 Hz), 110.9 (tquint, J = 270.8, 25.0 Hz), 112.0–119.0 (m, 2C for CF_2CF_2), 113.3, 114.3, 114.8, 118.7, 124.7 (t, J = 24.9 Hz), 129.9, 133.7, 144.3 (dd, J = 288.4, 14.3 Hz), 146.8 (dd, J = 293.8, 14.2 Hz), 146.4–147.2 (m), 161.0, 162.1, several carbon signals cannot be assigned due to extremely complex spin-spin coupling between carbon and fluorine atoms; ^{19}F NMR ($CDCl_3$): δ –111.13 (s, 4F), –132.44 (quint, J = 4.7 Hz, 2F), –135.5 (dd, J = 20.6, 10.9 Hz, 2F), –138.63 to –138.85 (m, 2F); IR (KBr): ν 3016, 2938, 2842, 2225, 1606, 1516, 1486, 1258, 1137, 1060, 996, 836 cm^{-1}; HRMS: (FAB+) *m/z* $[M]^+$ calcd for $C_{27}H_{14}F_{10}O_2$: 560.0834; found: 560.0844.

1.3. Typical synthetic procedure for 1-[2,3,5,6-Tetrafluoro-4-{2(4-methoxyphenyl)ethyn-1-yl}phenyl]-2-(2,3,4,5,6-pentafluorophenyl)-3,3,4,4,5,5-hexafluorocyclopentene (2bA): Path C

In at two-necked round-bottomed flask, equipped with a stirrer bar, was placed 4-methoxyphenyllithium (**8A**, 2.1 mmol), prepared from the reaction of 4-ethynylanisole (0.28 g, 2.1 mmol) and *n*-BuLi (1.6 mol L^{-1} hexane solution, 1.4 mL, 2.3 mmol) in THF at 0 °C for 0.5 h, and the whole was cooled to –78 °C. To the solution was added dropwise a THF (5.0 mL) solution of 1,2-bis(pentafluorophenyl)-3,3,4,4,5,5-hexafluorocyclopentene (**7**, 0.93 g, 1.8 mmol). After being stirred at 25 °C for 16 h, the resultant solution was poured into saturated aqueous NH_4Cl solution (20 mL), and the crude product was extracted with Et_2O (10 mL, three times) and organic layer was washed with brine (20 mL, once). Organic layer collected was dried over anhydrous Na_2SO_4, which was separated by atmospheric filtration. The filtrate was evaporated in vacuo and subjected to silica-gel column chromatography (eluent: hexane/EtOAc = 20/1), followed by recrystallization from CH_2Cl_2/MeOH (v/v = 1/1), to obtain the title compound **2bA** in 6% yield (0.066 g, 0.1 mmol) as a white solid.

*1.3.1. 1-[2,3,5,6-Tetrafluoro-4-{2(4-methoxyphenyl)ethyn-1-yl}phenyl]-2-(2,3,4,5,6-pentafluorophenyl)-3,3,4,4,5,5-hexafluorocyclopentene (**2bA**)*

Yield: 6% (white solid); m.p.: 118.4–119.6 °C; ^{1}H NMR ($CDCl_3$): 3.85 (s, 3H), 6.91 (d, J = 8.8 Hz, 2H), 7.52 (d, J = 8.8

Hz, 2H); ^{13}C NMR ($CDCl_3$): δ 55.4, 72.8 (t, *J* = 4.4 Hz), 101.4 (td, *J* = 18.9, 3.7 Hz), 104.7 (t, *J* = 19.1 Hz), 105.5 (t, *J* = 2.9 Hz), 109.2 (t, *J* = 17.6 Hz), 110.7 (tquint, *J* = 275.1, 25.8 Hz), 113.0, 114.3, 114.5 (tt, *J* = 261.9, 23.8 Hz), 133.8, 136.1 (t, *J* = 26.3 Hz), 137.5 (t, *J* = 31.5 Hz), 137.9 (dtd, *J* = 253.7, 13.2, 5.1 Hz), 141.7–145.0 (dm, *J* = 261.1 Hz), 143.7 (ddt, *J* = 253.8, 14.6, 4.4 Hz), 143.0–145.7 (dm, *J* = 250.8 Hz), 146.6 (ddt, *J* = 255.2, 13.9, 4.4 Hz), 161.2, one carbon signals cannot be assigned due to extremely complex spin-spin coupling between carbon and fluorine atoms; 19F NMR (CDCl3): d –111.88 (s, 2F), –112.03 (s, 2F), –132.65 (brs, 2F), –134.7 to –134.9 (m, 2F), –136.8 to –137.04 (m, 2F), –138.56 to –138.78 (m, 2F), –146.88 (t, *J* = 19.2 Hz, 1F), –158.57 to –158.83 (m, 2F); IR (KBr): ν 3024, 2949, 2847, 2226, 1605, 1520, 1486, 1247, 1163, 1034, 991, 835 cm^{-1}; HRMS: (FAB+) *m/z* $[M]^+$ calcd for $C_{26}H_7F_{15}O$: 620.0257; found: 620.0247.

*1.3.2. 1-[2,3,5,6-Tetrafluoro-4-{2(4-ethoxyphenyl)ethyn-1-yl}phenyl]-2-(2,3,4,5,6-pentafluorophenyl)-3,3,4,4,5,5-hexafluorocyclopentene (**2bB**)*

Yield: 22% (white solid); m.p.: 148.6–149.6 °C; ^{1}H NMR ($CDCl_3$): δ 1.44 (t, *J* = 7.2 Hz, 3H), 4.07 (q, *J* = 7.2 Hz, 2H), 6.90 (d, *J* = 8.8 Hz, 2H), 7.51 (d, *J* = 8.8 Hz, 2H); ^{13}C NMR ($CDCl_3$): δ 14.6, 63.7, 72.7 (t, *J* = 4.4 Hz), 101.4 (t, *J* = 19.8 Hz), 104.7 (d, *J* = 18.3 Hz), 105.6 (t, *J* = 3.6 Hz), 109.2 (t, *J* = 17.6 Hz), 110.7 (tquint, *J* = 273.5, 24.9 Hz), 112.8, 114.5 (tt, *J* = 261.6, 24.1 Hz), 114.8, 133.8, 136.1 (t, *J* = 27.2 Hz), 137.6 (t, *J* = 25.6 Hz), 137.9 (dtd, *J* = 253.8, 14.0, 5.9 Hz), 143.3 (dtt, *J* = 261.2, 13.3, 4.4 Hz), 143.7 (ddt, *J* = 254.4, 14.6, 4.3 Hz), 143.0–145.8 (dm, *J* = 256.0 Hz), 146.6 (ddt, *J* = 255.2, 14.0, 4.4 Hz), 160.6, one carbon signals cannot be assigned due to extremely complex spin-spin coupling between carbon and fluorine atoms; ^{19}F NMR ($CDCl_3$): δ –111.88 (s, 2F), –112.03 (s, 2F), –132.65 (quint, *J* = 3.8 Hz, 2F), –134.82 (dd, *J* = 19.5, 9.9 Hz, 2F), –136.80 to –137.03 (m, 2F), –138.57 to –138.82 (m, 2F), –146.89 (t, *J* = 21.8 Hz, 1F), –158.70 (td, *J* = 20.3, 5.3 Hz, 2F); IR (KBr): ν 2998, 2884, 2221, 1603, 1519, 1359, 1252, 1064, 995, 838 cm^{-1}; HRMS: (FAB+) *m/z* $[M]^+$ calcd for $C_{27}H_9F_{15}O$: 634.0414; found: 634.0430.

2. NMR spectra

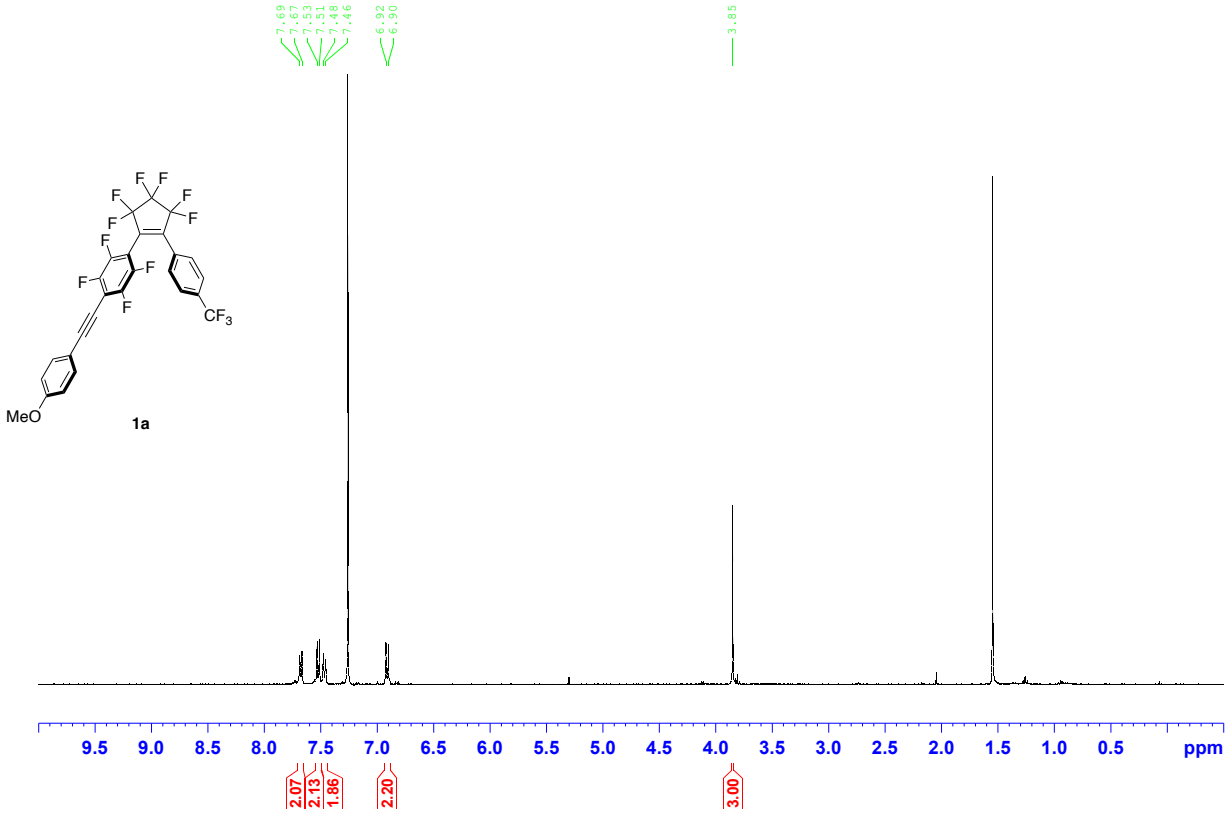


Figure S2. ^{1}H NMR spectrum of **1a** ($CDCl_3$, 400 MHz)

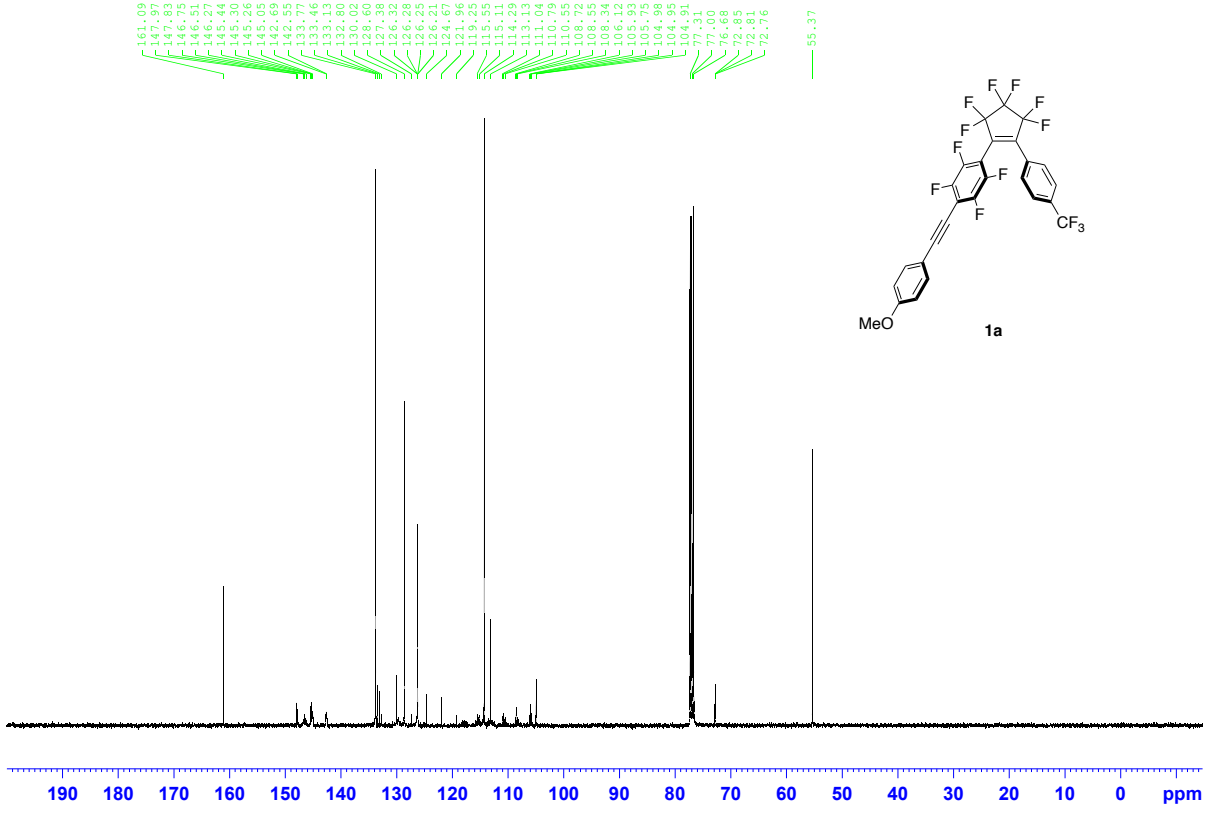


Figure S3. ^{13}C NMR spectrum of **1a** ($CDCl_3$, 100 MHz)

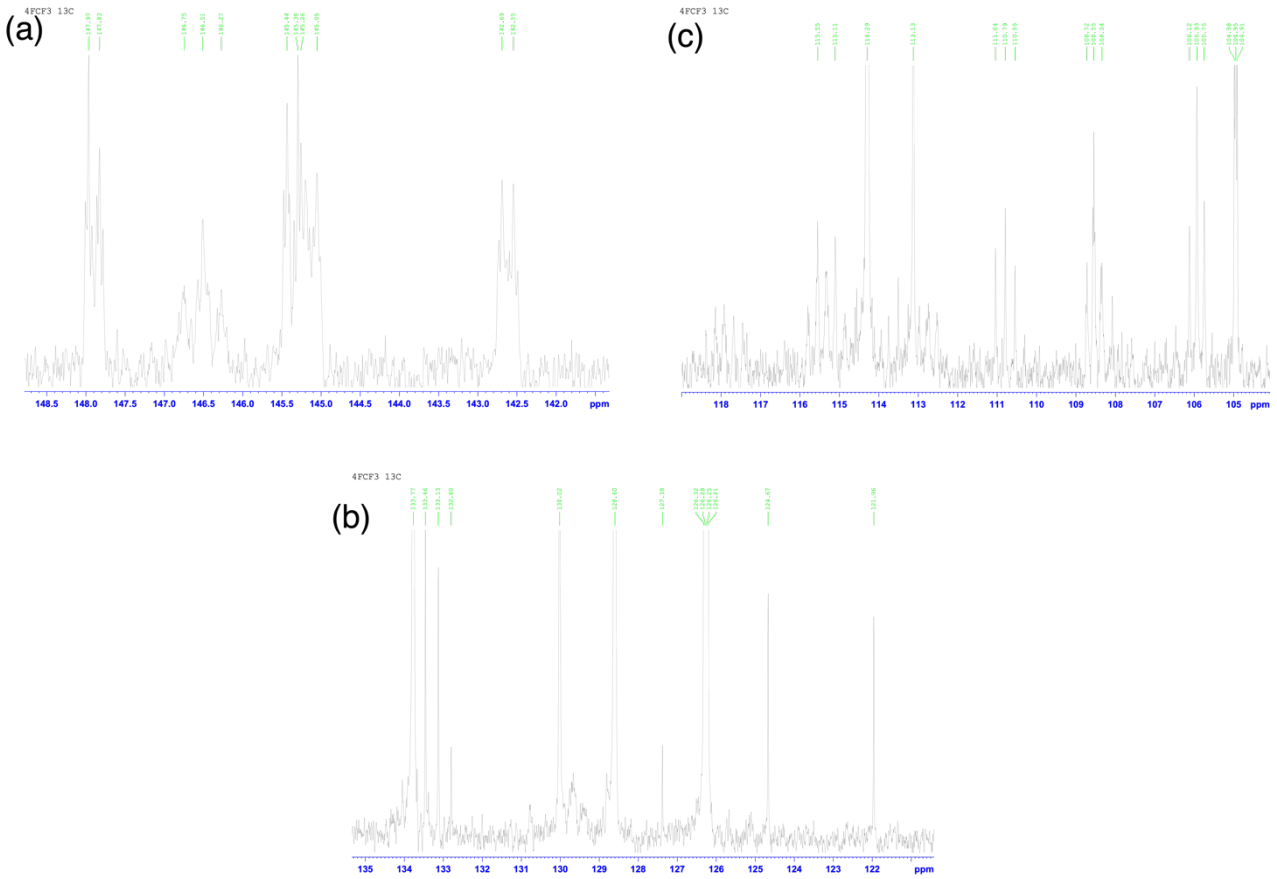


Figure S4. Expansion of ^{13}C NMR spectrum of **1a**: (a) 149–142 ppm; (b) 135–120 ppm; (c) 120–104 ppm.

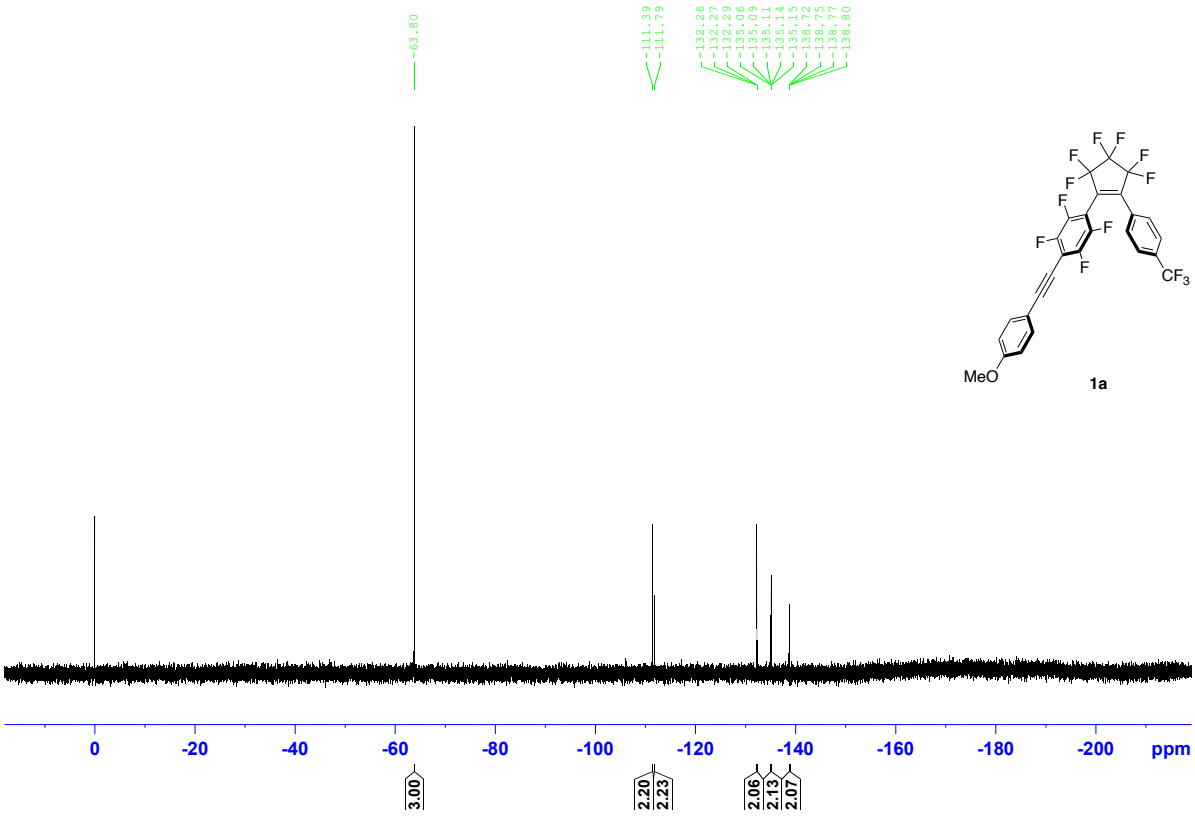


Figure S5. ^{19}F NMR spectrum of **1a** ($CDCl_3$, 376 MHz)

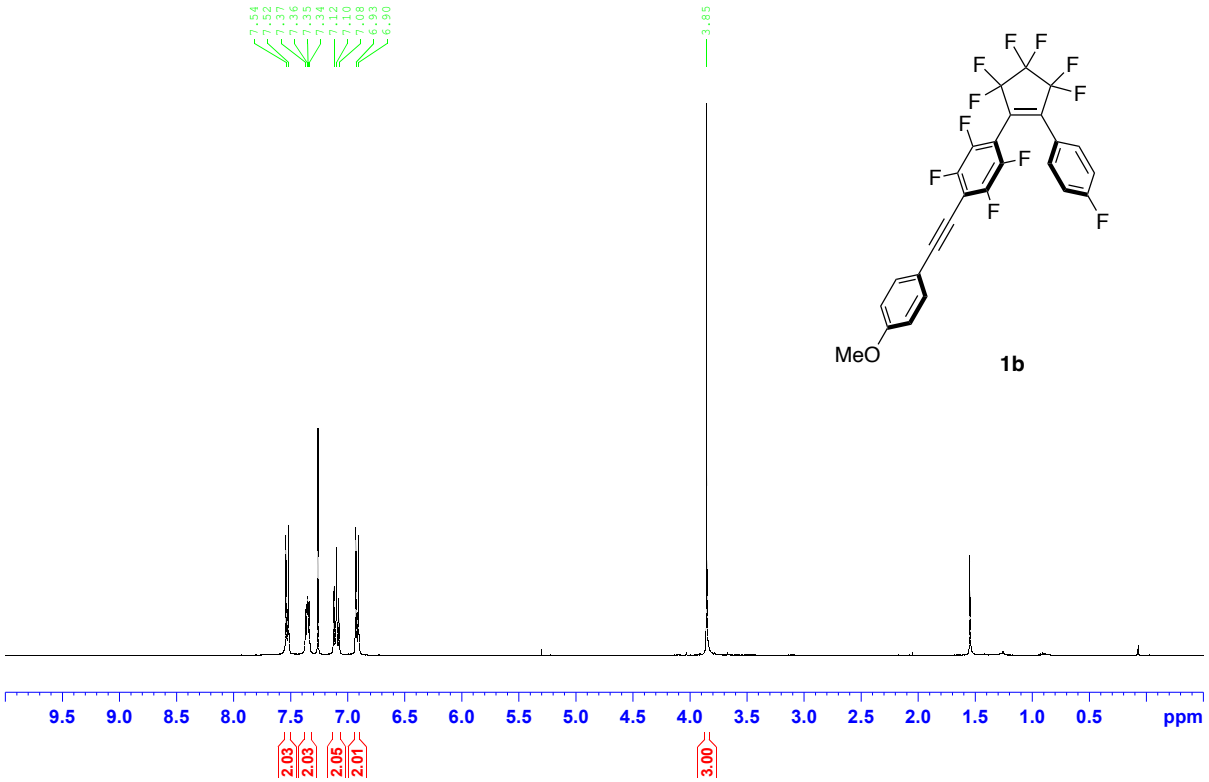


Figure S6. ^{1}H NMR spectrum of **1b** ($CDCl_3$, 400 MHz)

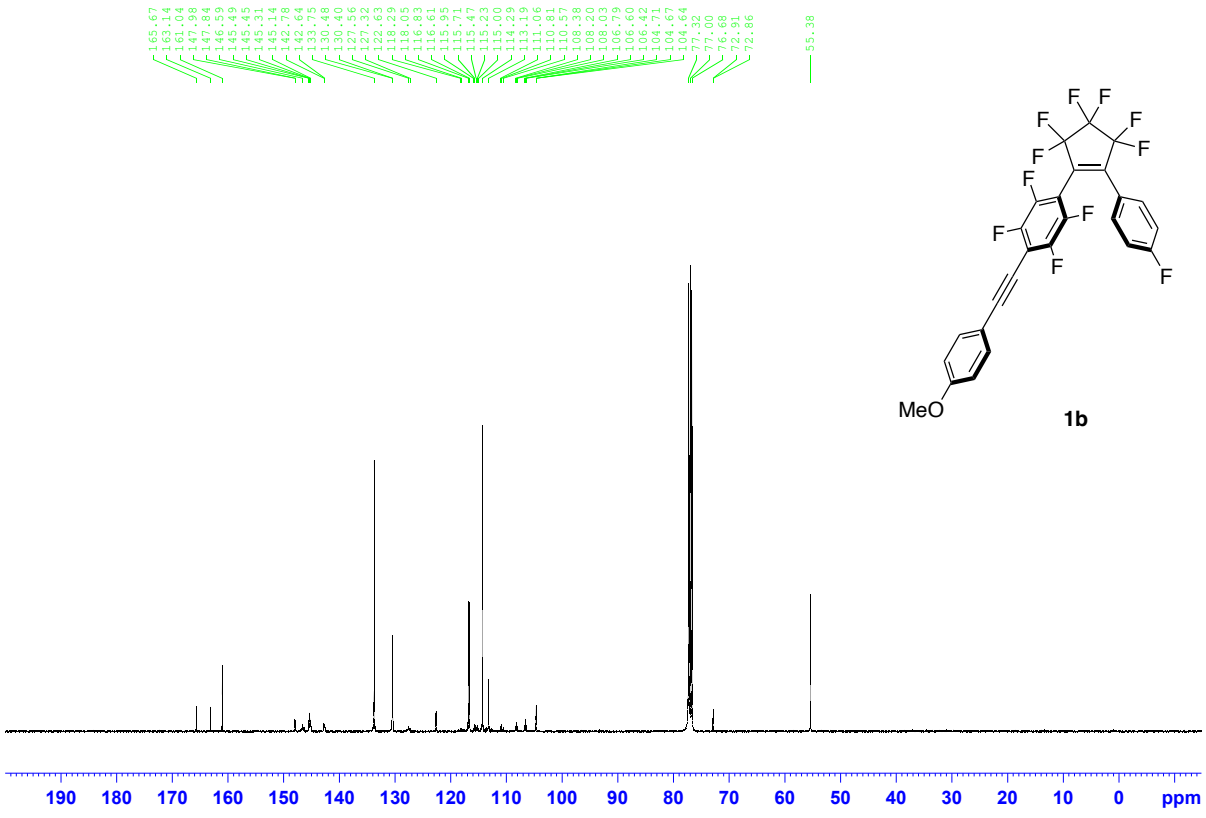


Figure S7. ^{13}C NMR spectrum of **1b** ($CDCl_3$, 100 MHz)

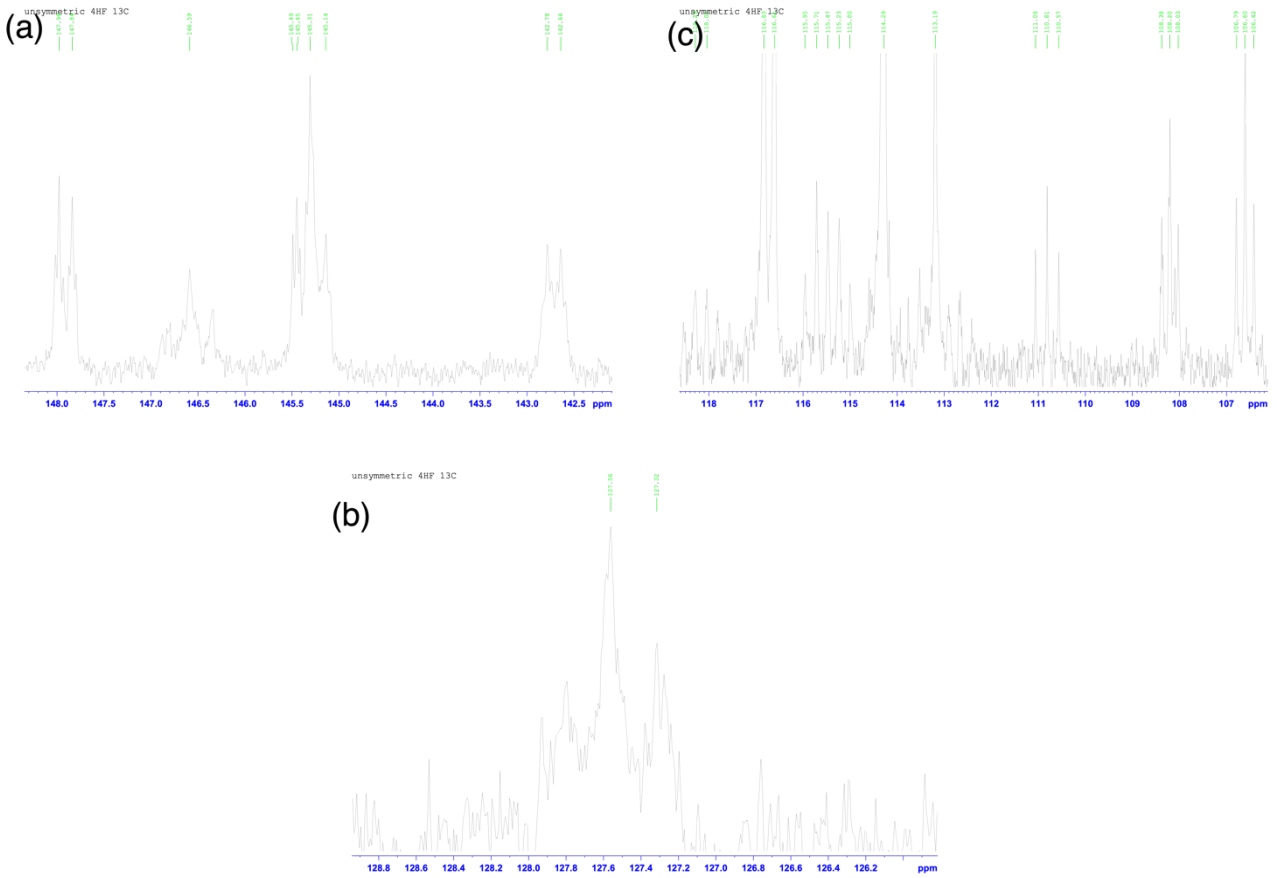


Figure S8. Expansion of ^{13}C NMR spectrum of **1b**: (a) 149–142 ppm; (b) 128–120 ppm; (c) 120–104 ppm.

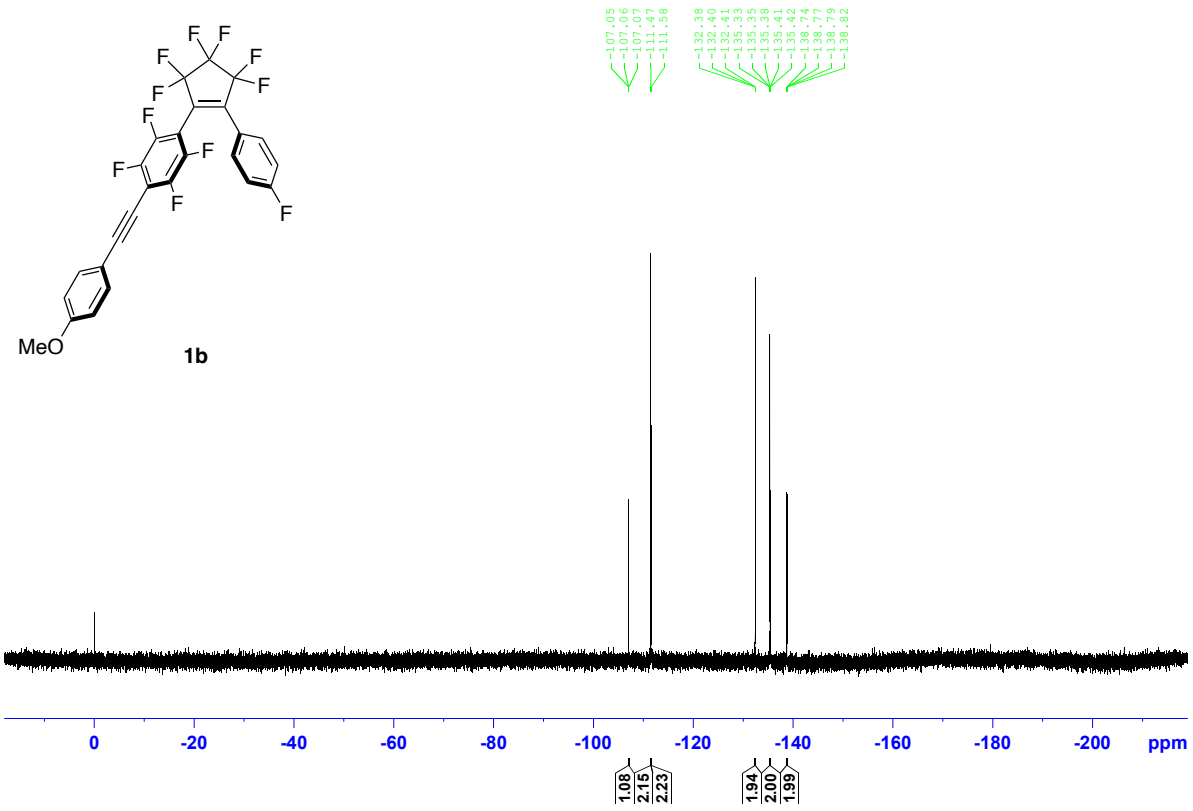


Figure S9. ^{19}F NMR spectrum of **1b** ($CDCl_3$, 376 MHz)

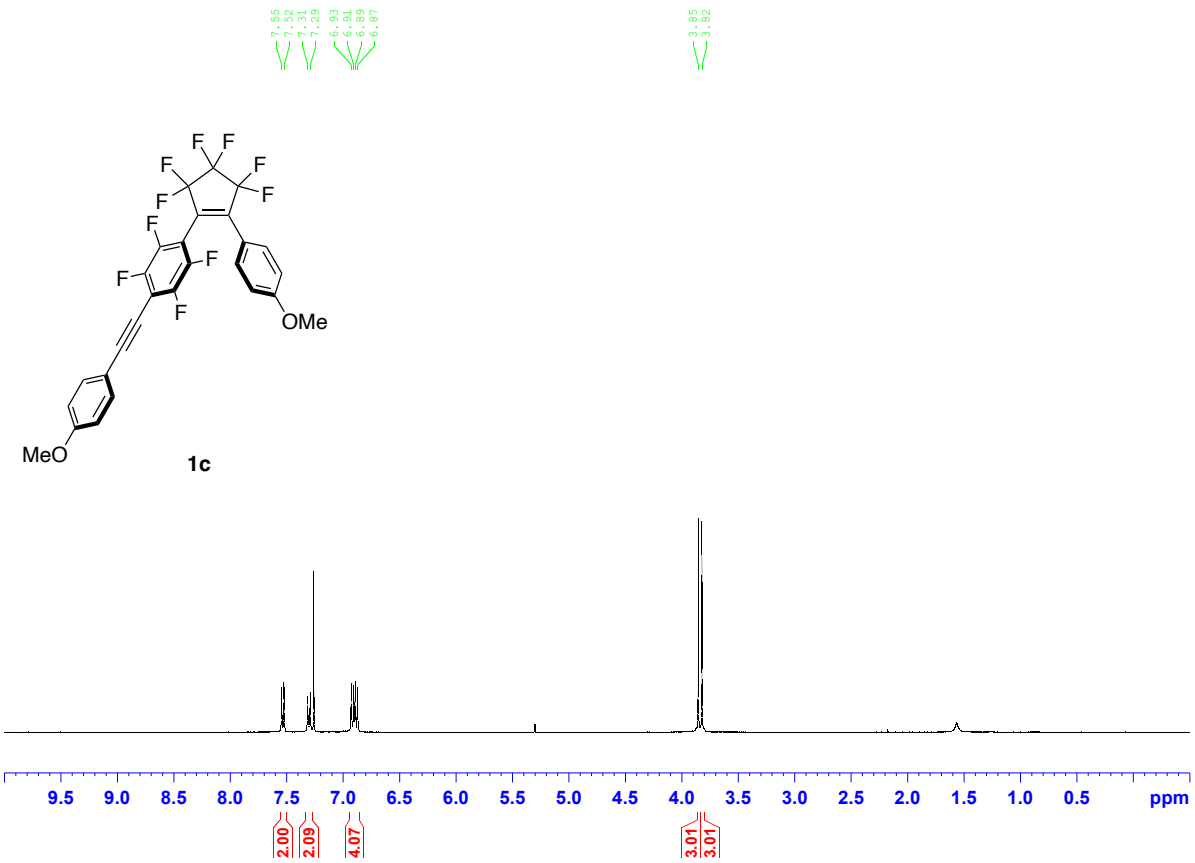


Figure S10. ^{1}H NMR spectrum of **1c** ($CDCl_3$, 400 MHz)

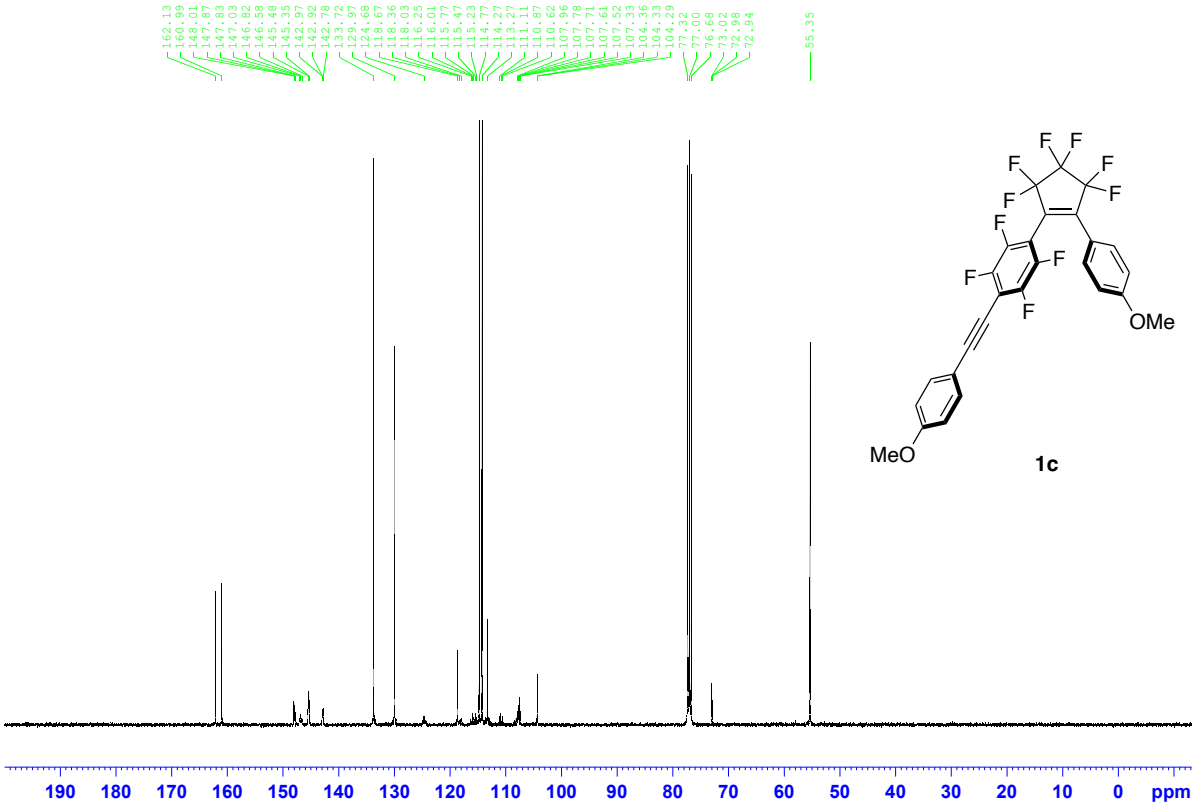


Figure S11. ^{13}C NMR spectrum of **1c** ($CDCl_3$, 400 MHz)

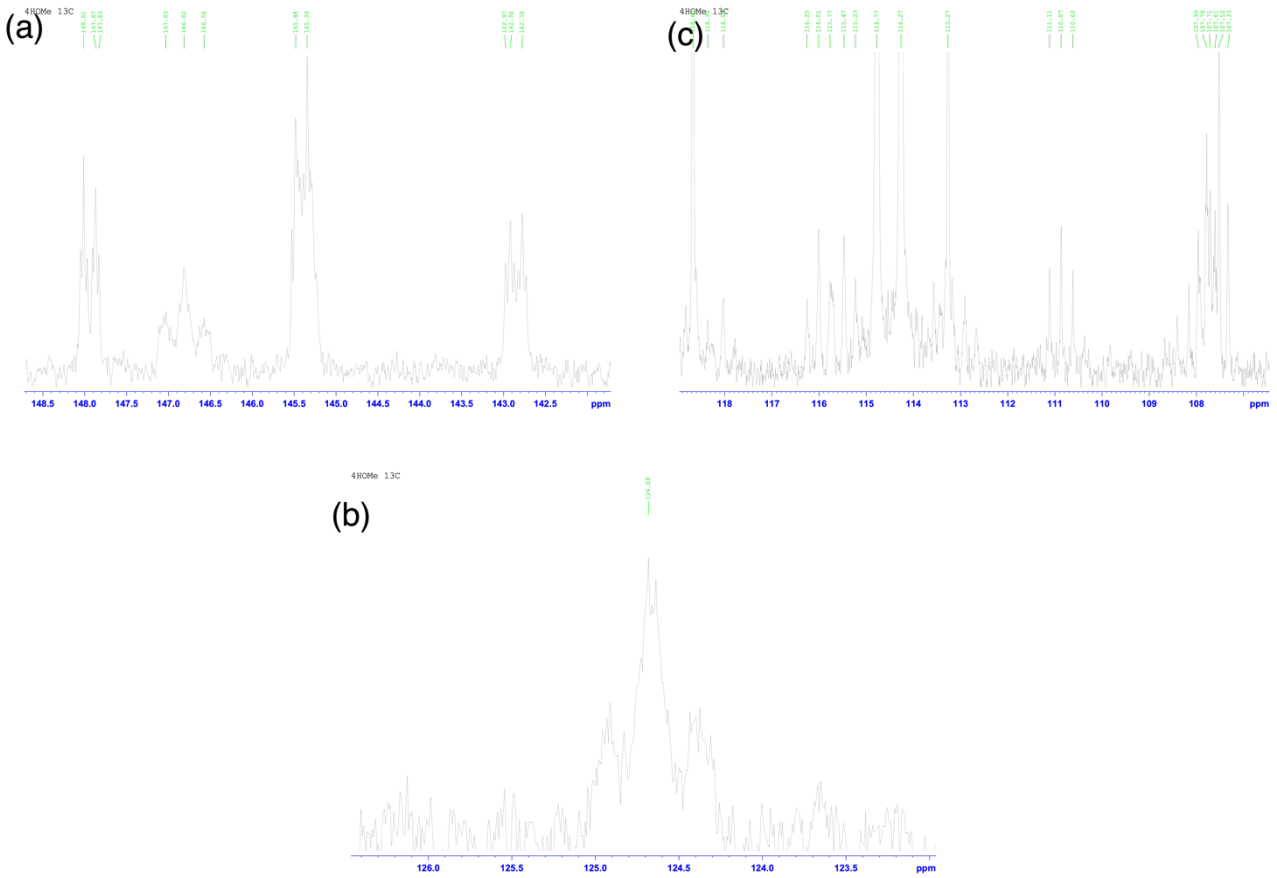


Figure S12. Expansion of ^{13}C NMR spectrum of **1c**: (a) 149–142 ppm; (b) 128–120 ppm; (c) 120–104 ppm.

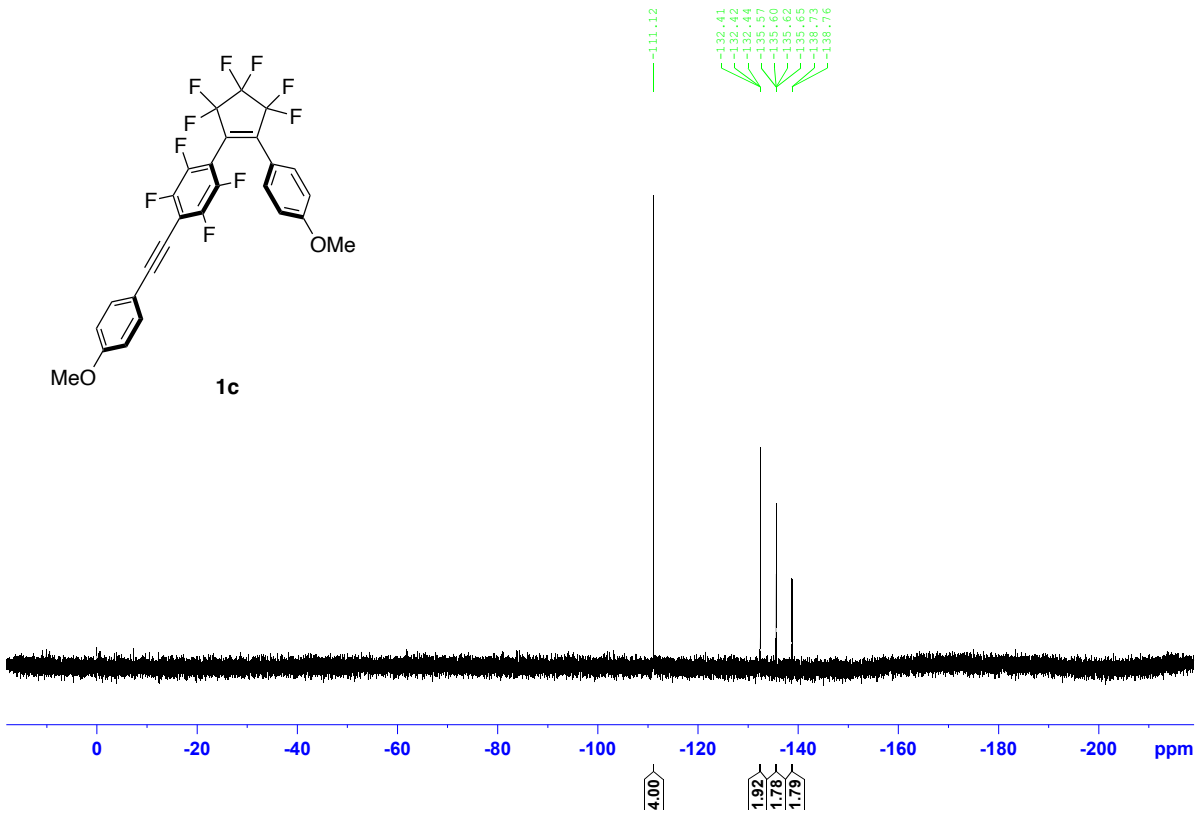


Figure S13. ^{19}F NMR spectrum of **1c** ($CDCl_3$, 400 MHz)

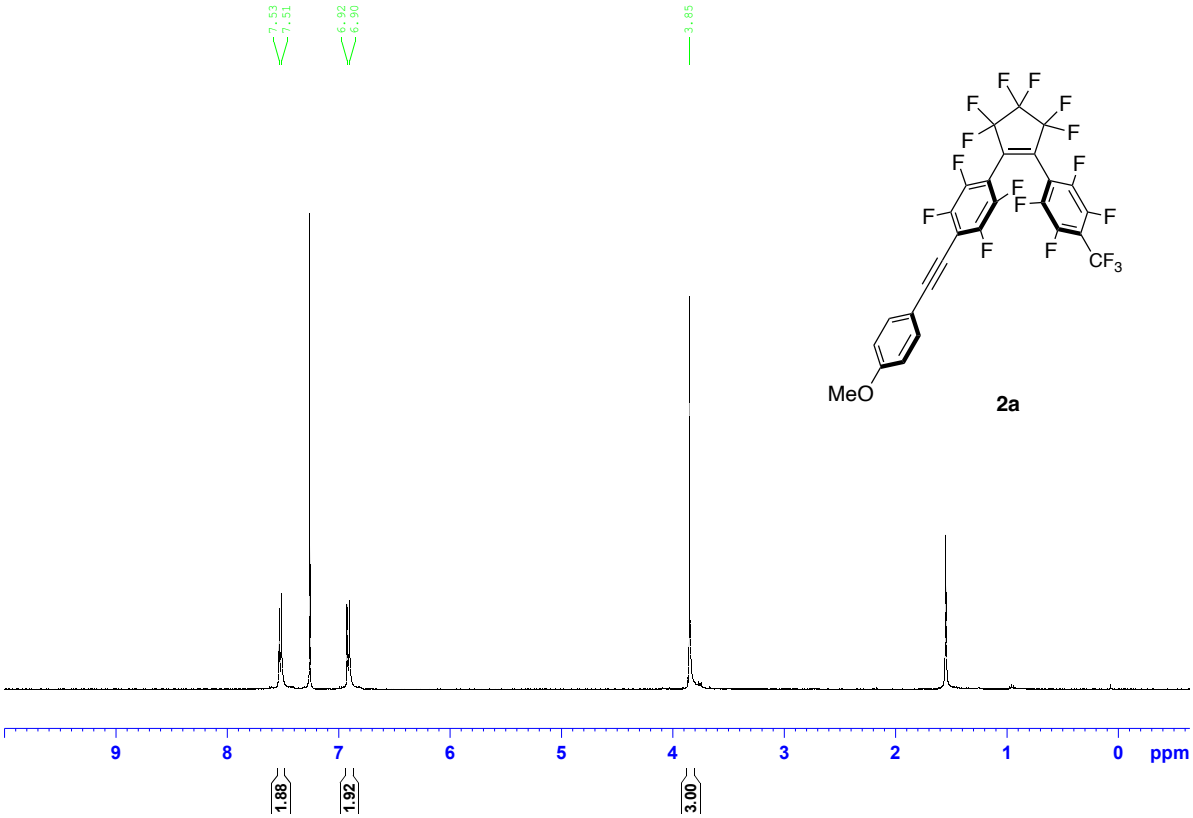


Figure S14. ^{1}H NMR spectrum of **2a** ($CDCl_3$, 400 MHz)

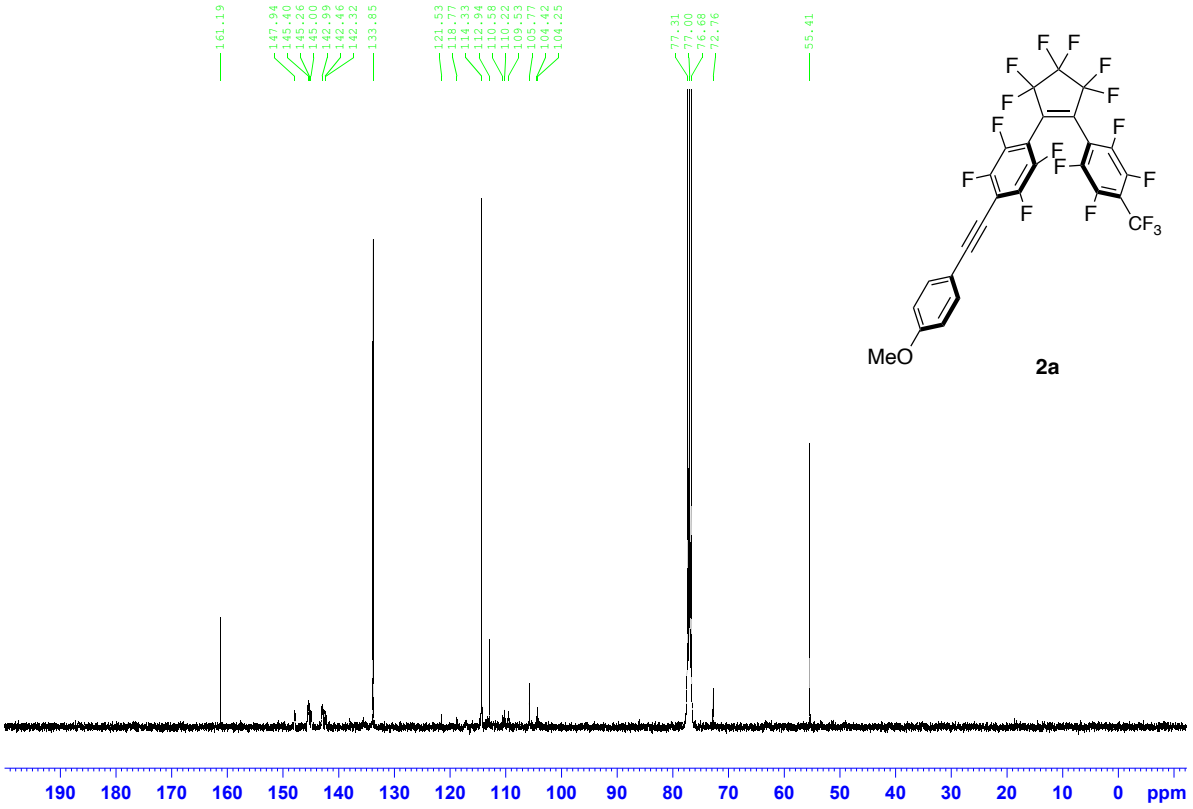


Figure S15. ^{13}C NMR spectrum of **2a** ($CDCl_3$, 100 MHz)

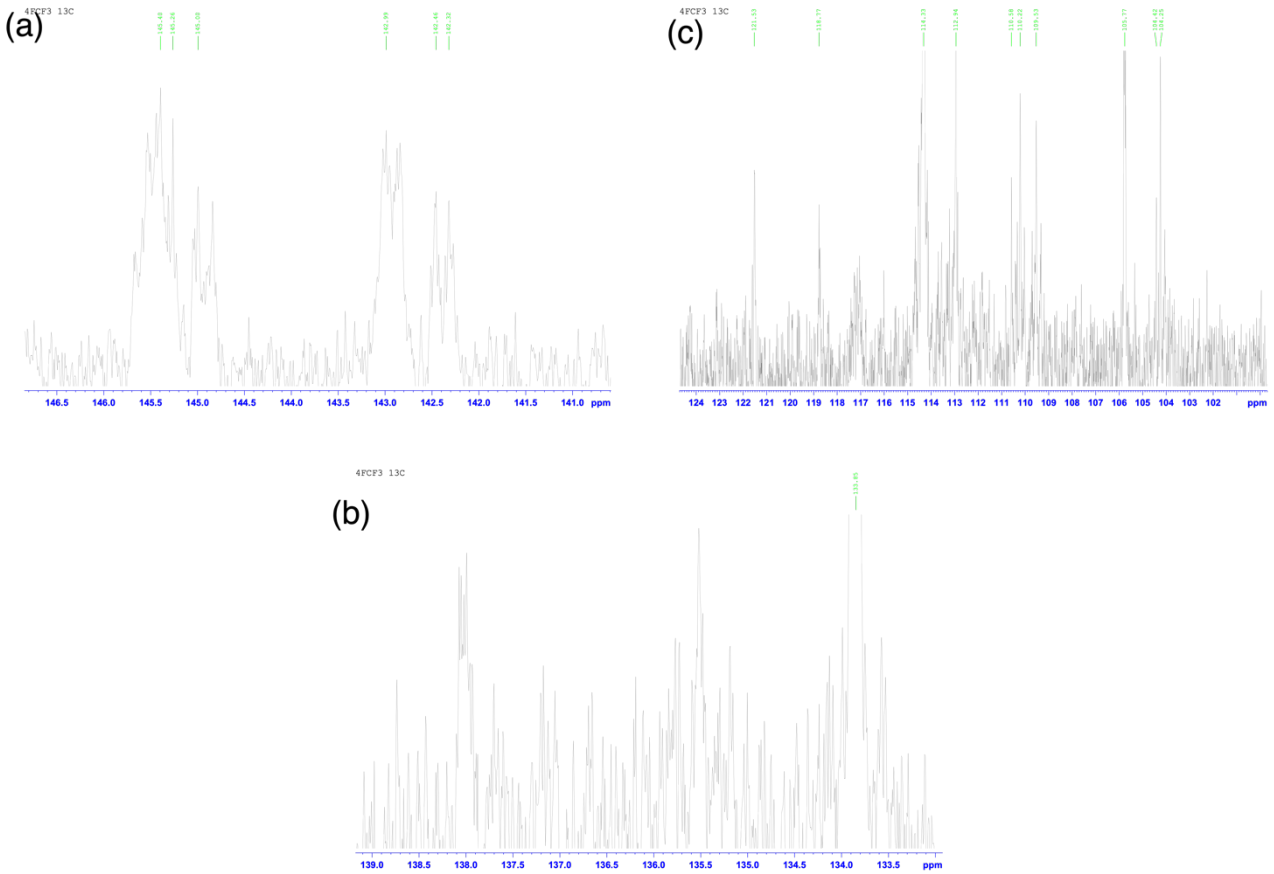


Figure S16. Expansion of ^{13}C NMR spectrum of **2a**: (a) 147–141 ppm; (b) 139–133 ppm; (c) 125–100 ppm.

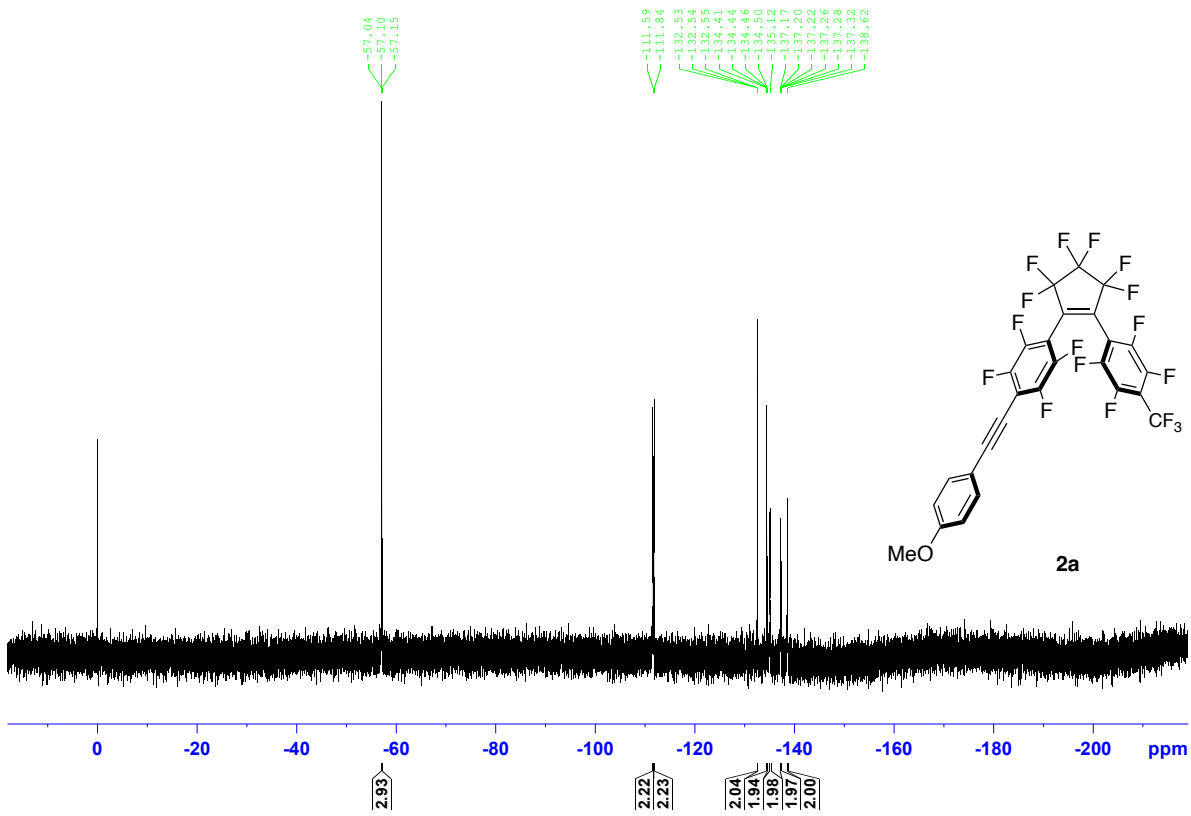


Figure S17. ^{19}F NMR spectrum of **2a** ($CDCl_3$, 376 MHz)

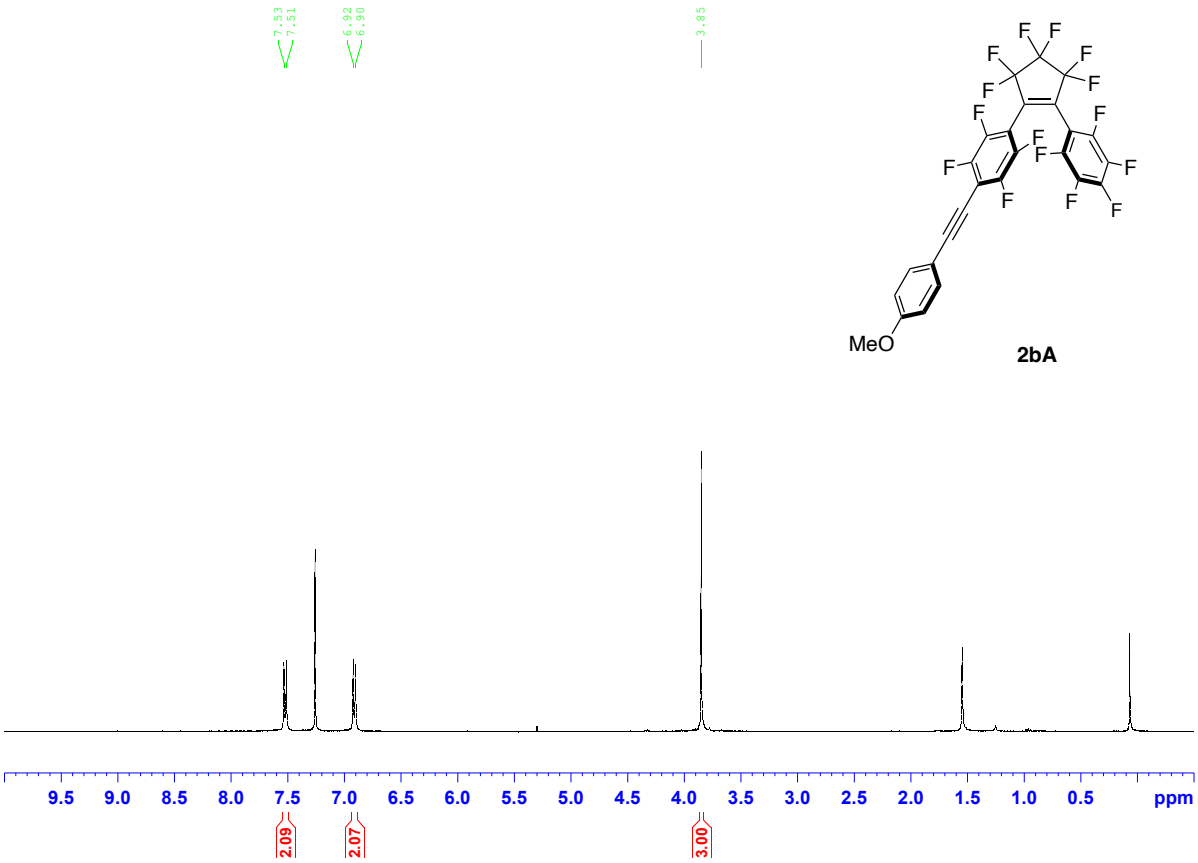


Figure S18. ^{1}H NMR spectrum of **2bA** ($CDCl_3$, 400 MHz)

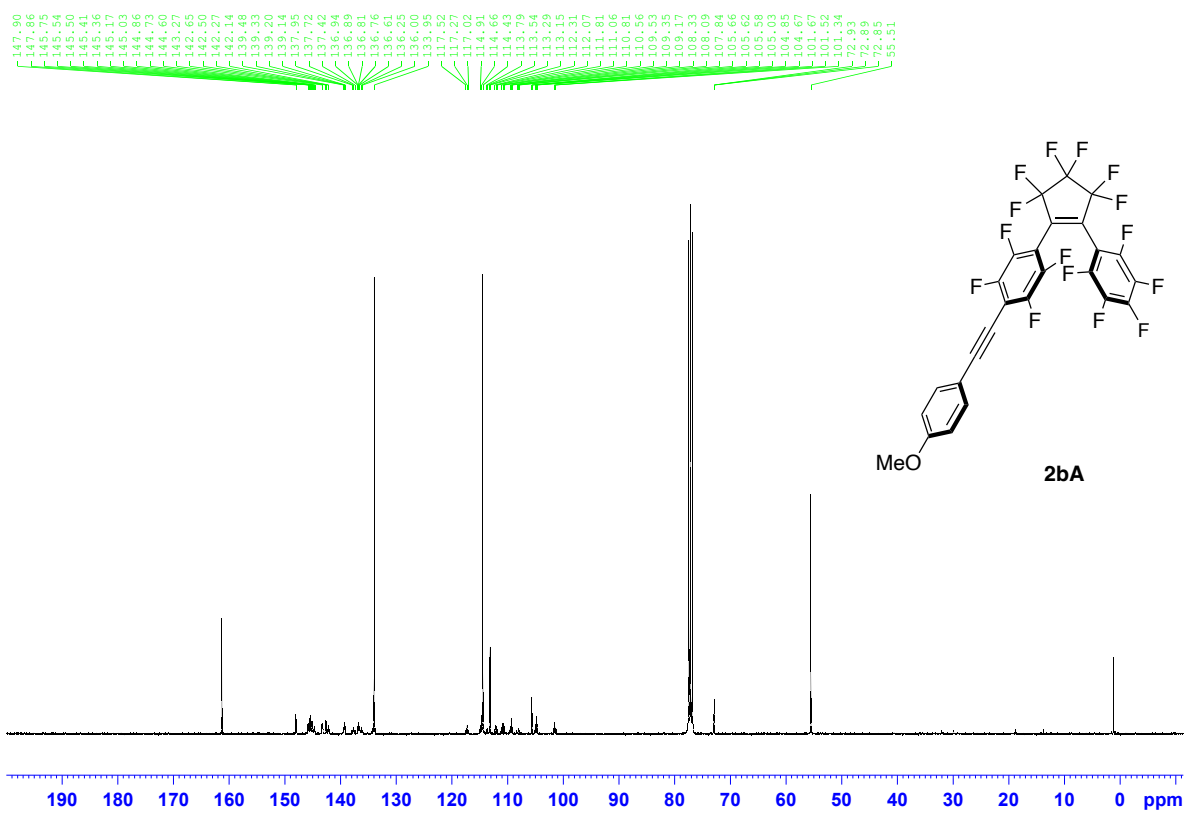


Figure S19. ^{13}C NMR spectrum of **2bA** ($CDCl_3$, 100 MHz)

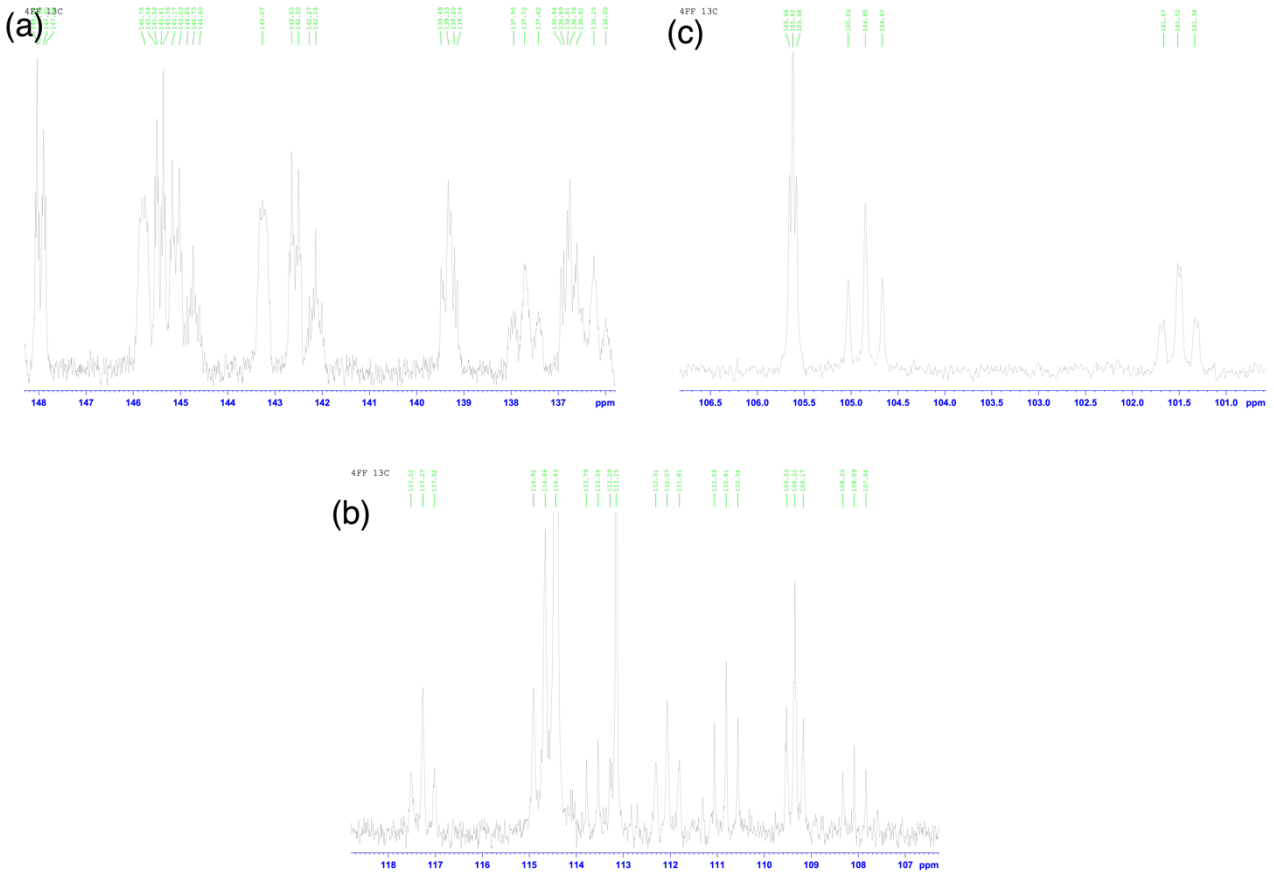


Figure S20. Expansion of ^{13}C NMR spectrum of **2bA**: (a) 148–136 ppm; (b) 118–107 ppm; (c) 107–101 ppm.

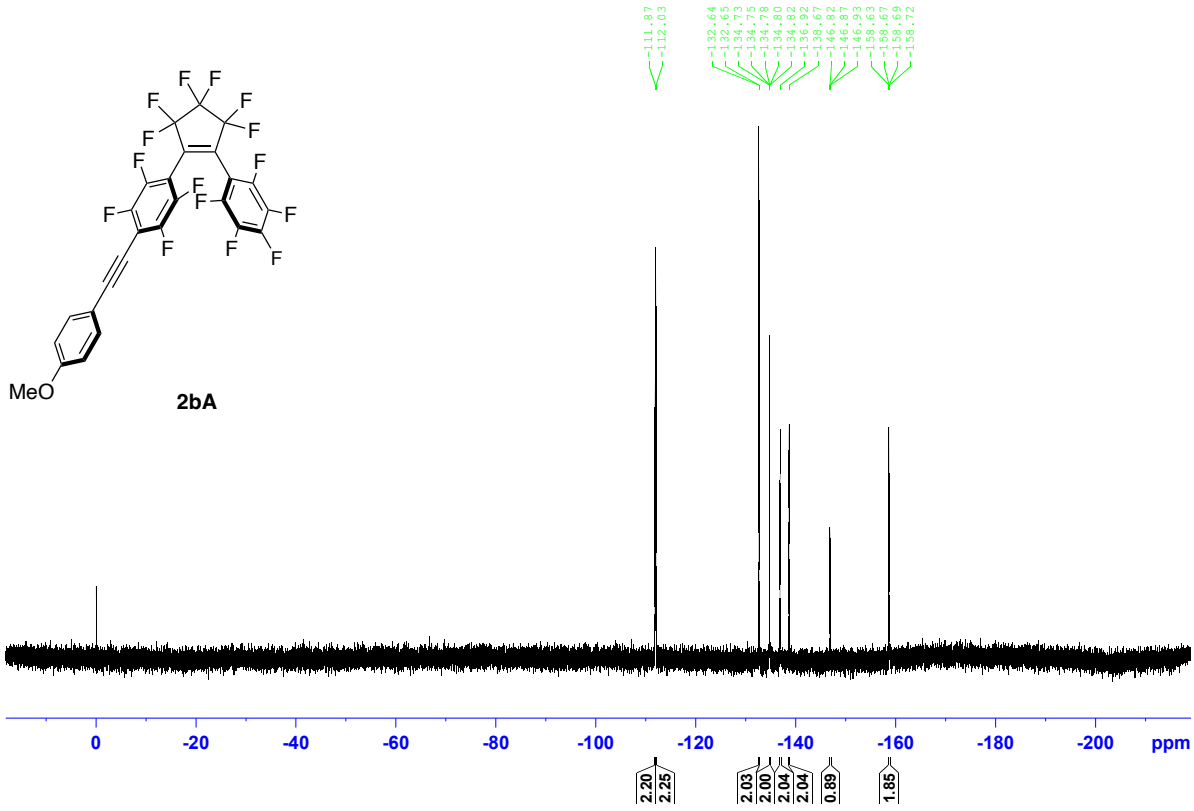


Figure S21. ^{19}F NMR spectrum of **2bA** ($CDCl_3$, 376 MHz)

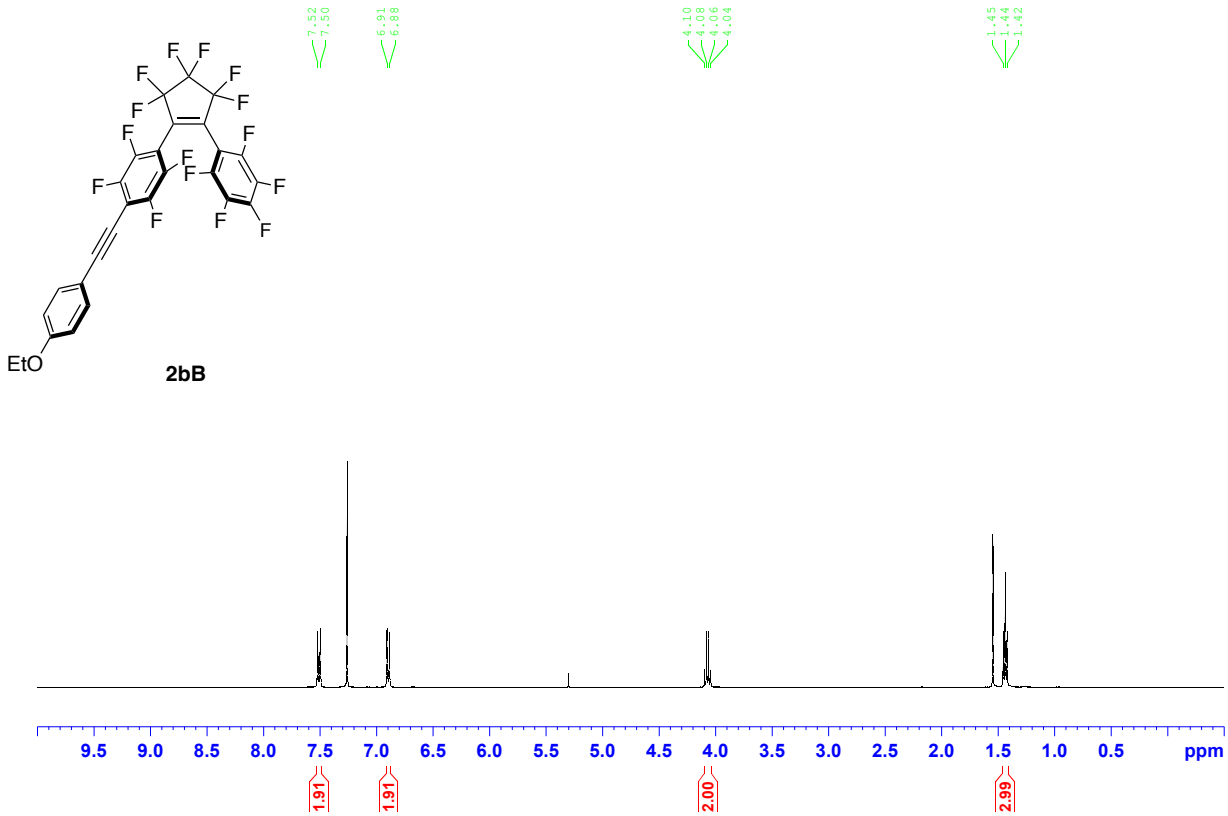


Figure S22. ^{1}H NMR spectrum of **2bB** ($CDCl_3$, 400 MHz)

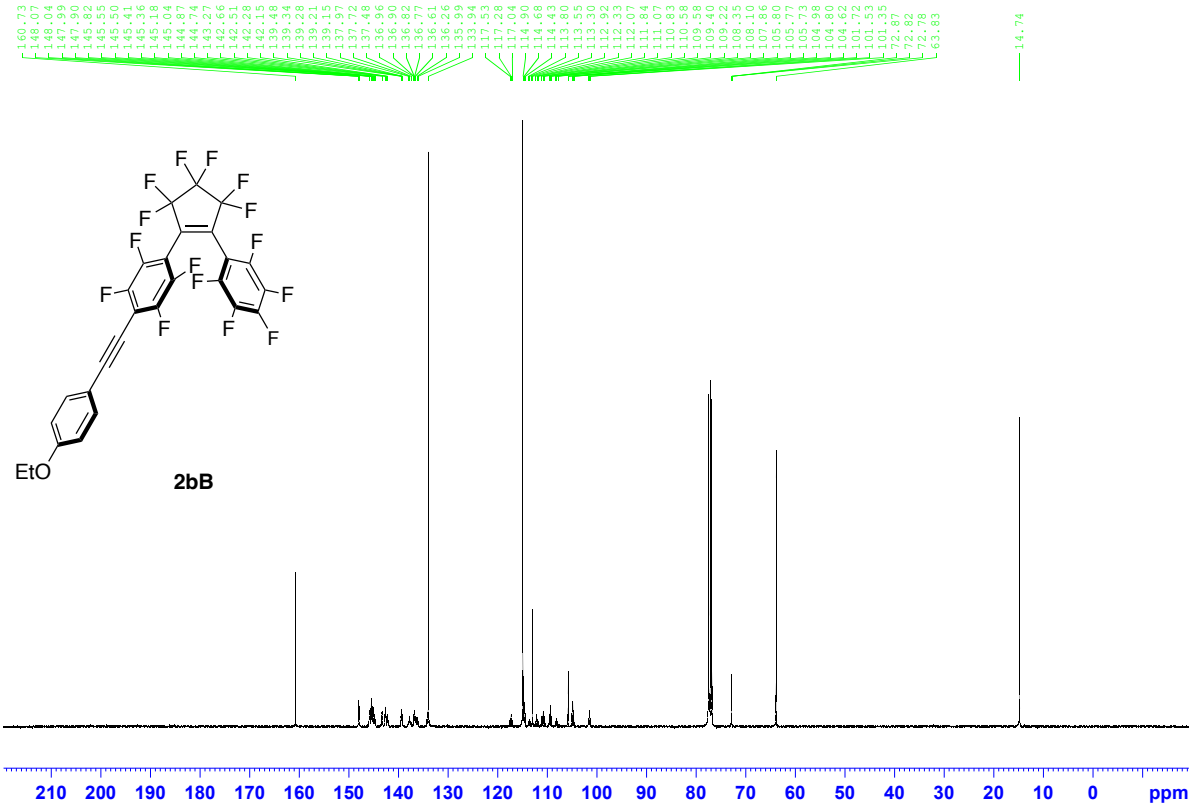


Figure S23. ^{13}C NMR spectrum of **2bB** ($CDCl_3$, 100 MHz)

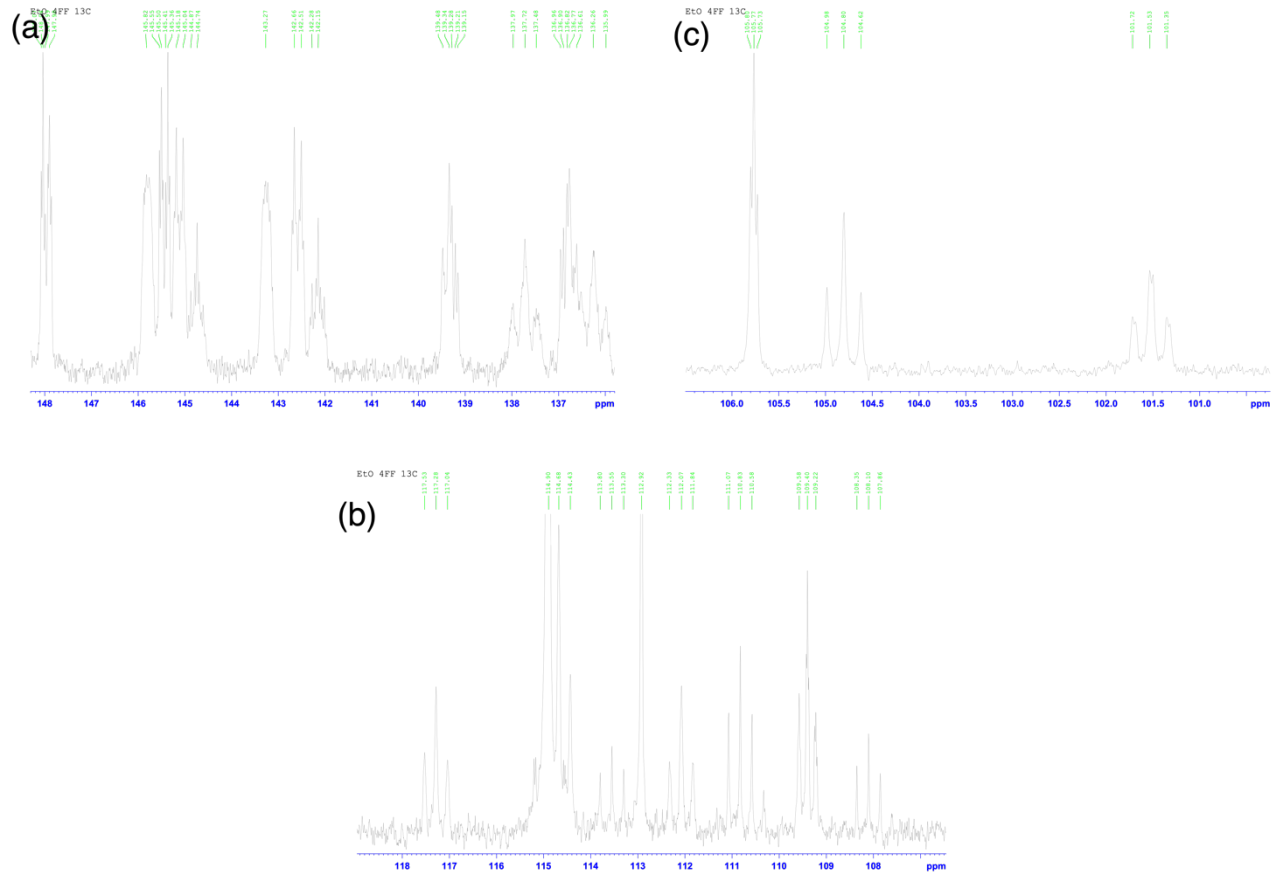


Figure S24. Expansion of ^{13}C NMR spectrum of **2bB**: (a) 148–136 ppm; (b) 118–107 ppm; (c) 107–101 ppm.

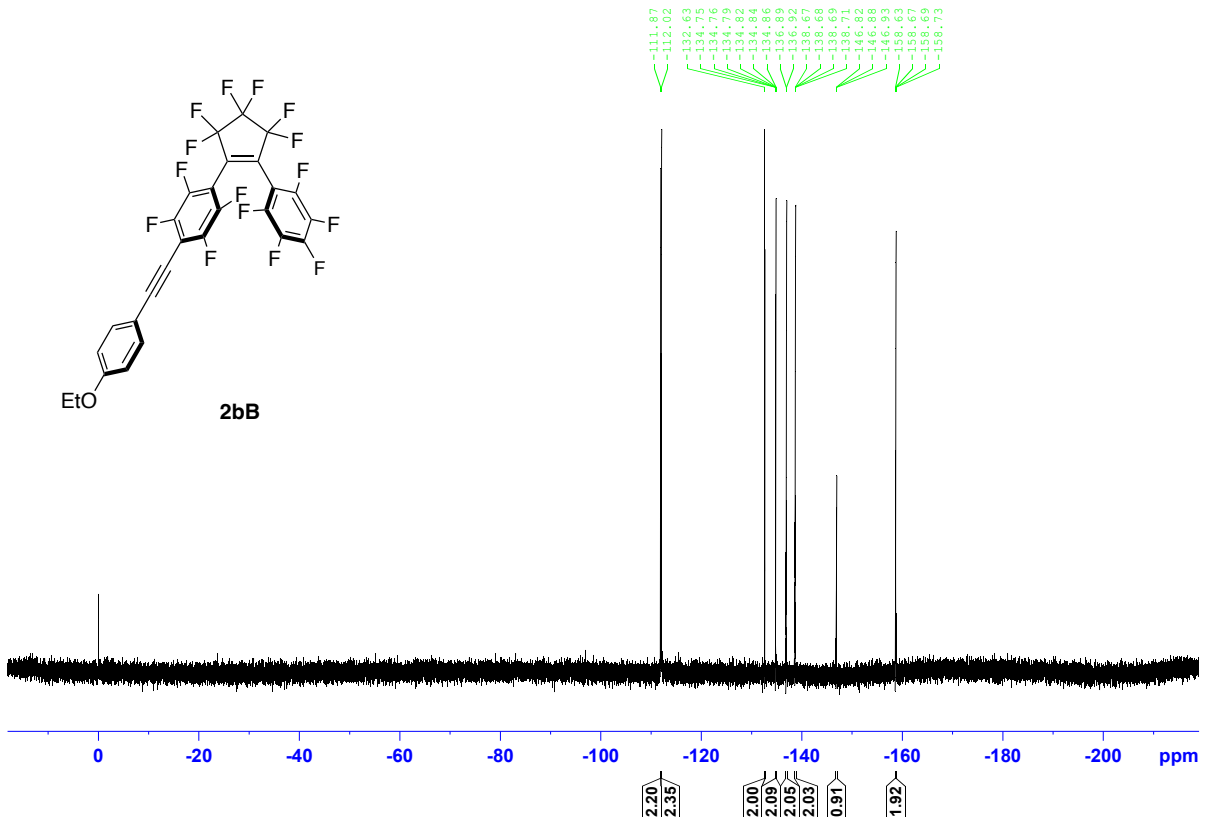


Figure S25. ^{19}F NMR spectrum of **2bB** ($CDCl_3$, 376 MHz)

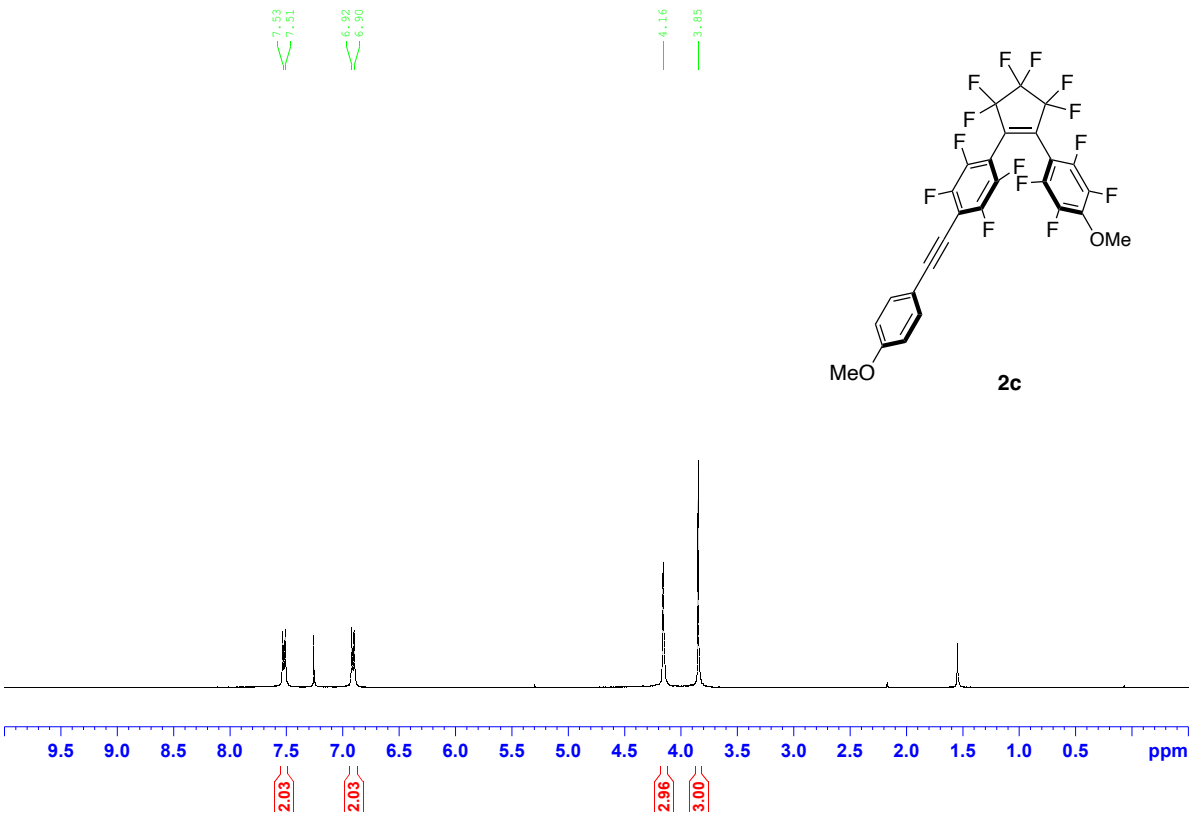


Figure S26. ^{1}H NMR spectrum of **2c** ($CDCl_3$, 400 MHz)

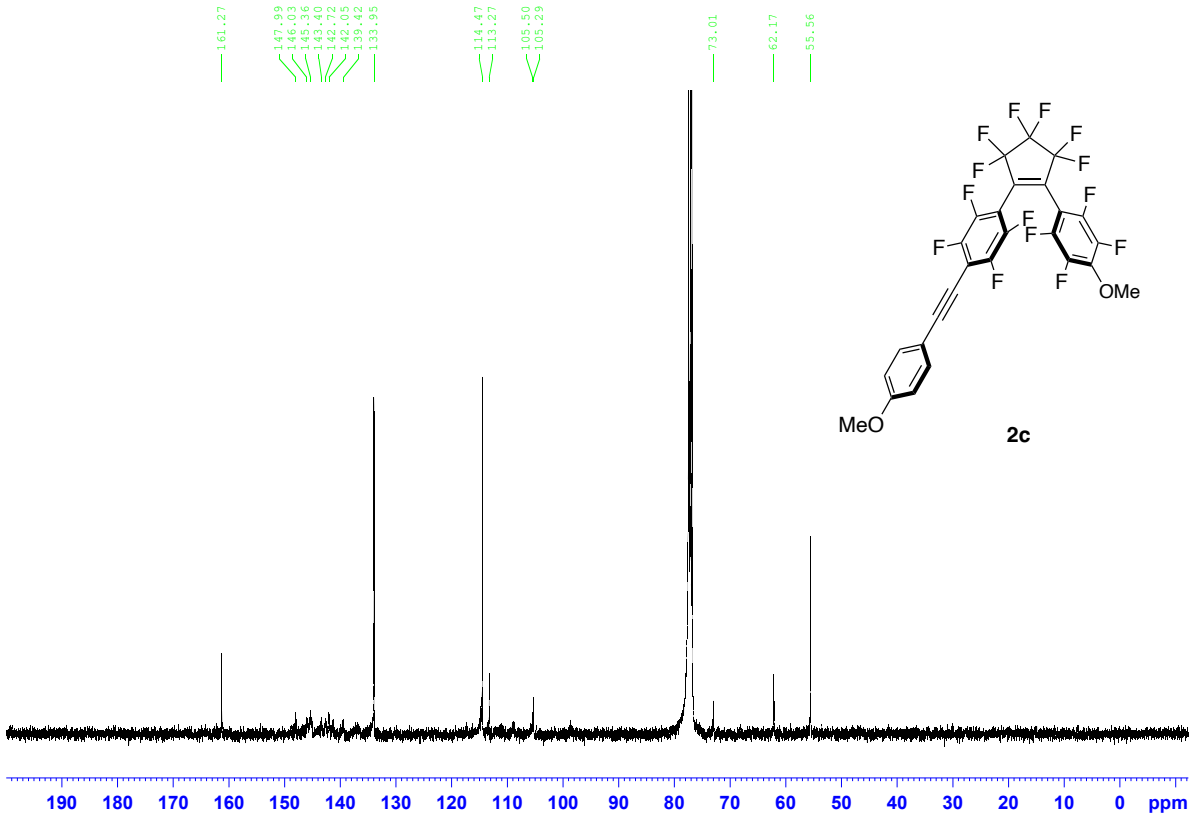


Figure S27. ^{13}C NMR spectrum of **2c** ($CDCl_3$, 100 MHz)

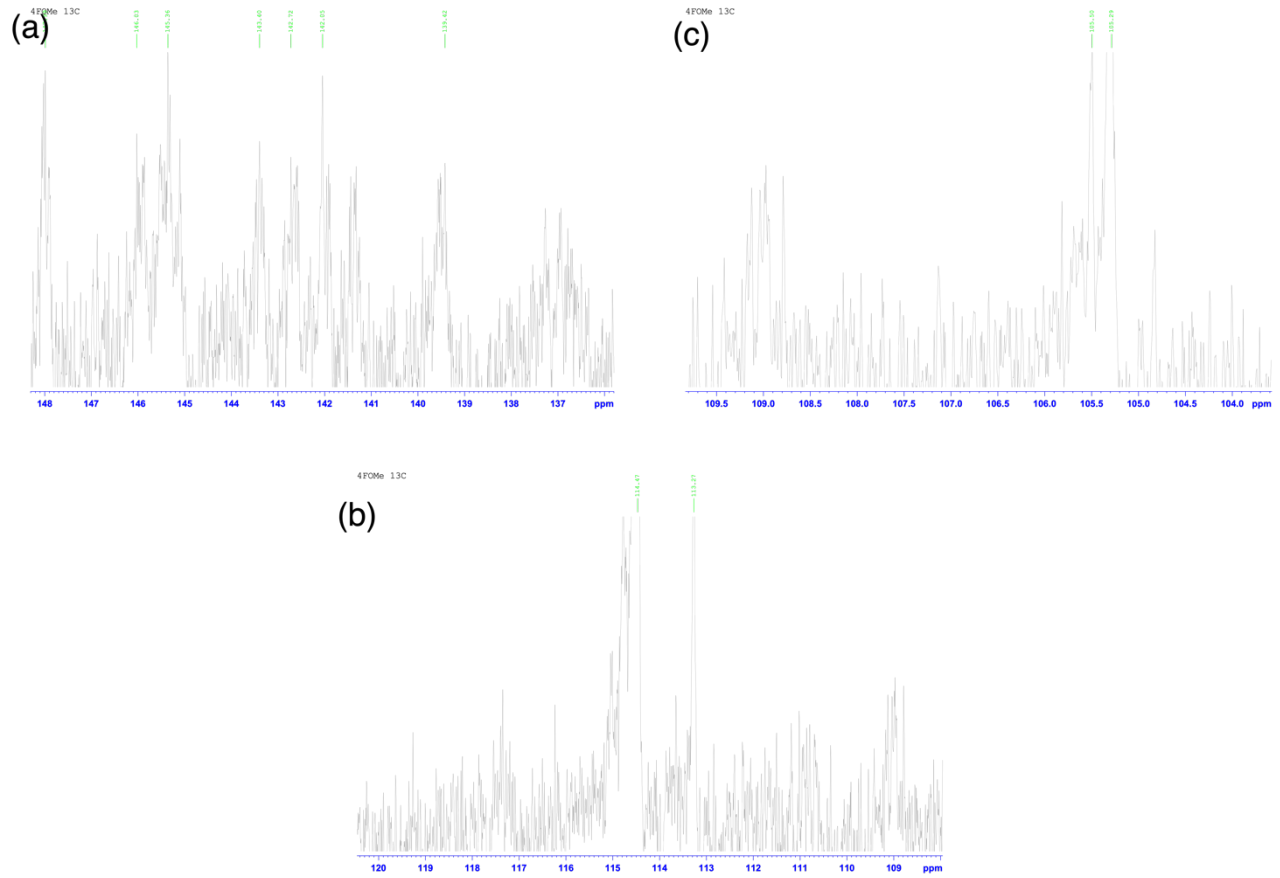


Figure S28. Expansion of ^{13}C NMR spectrum of **2c**: (a) 148–136 ppm; (b) 120–108 ppm; (c) 110–103 ppm.

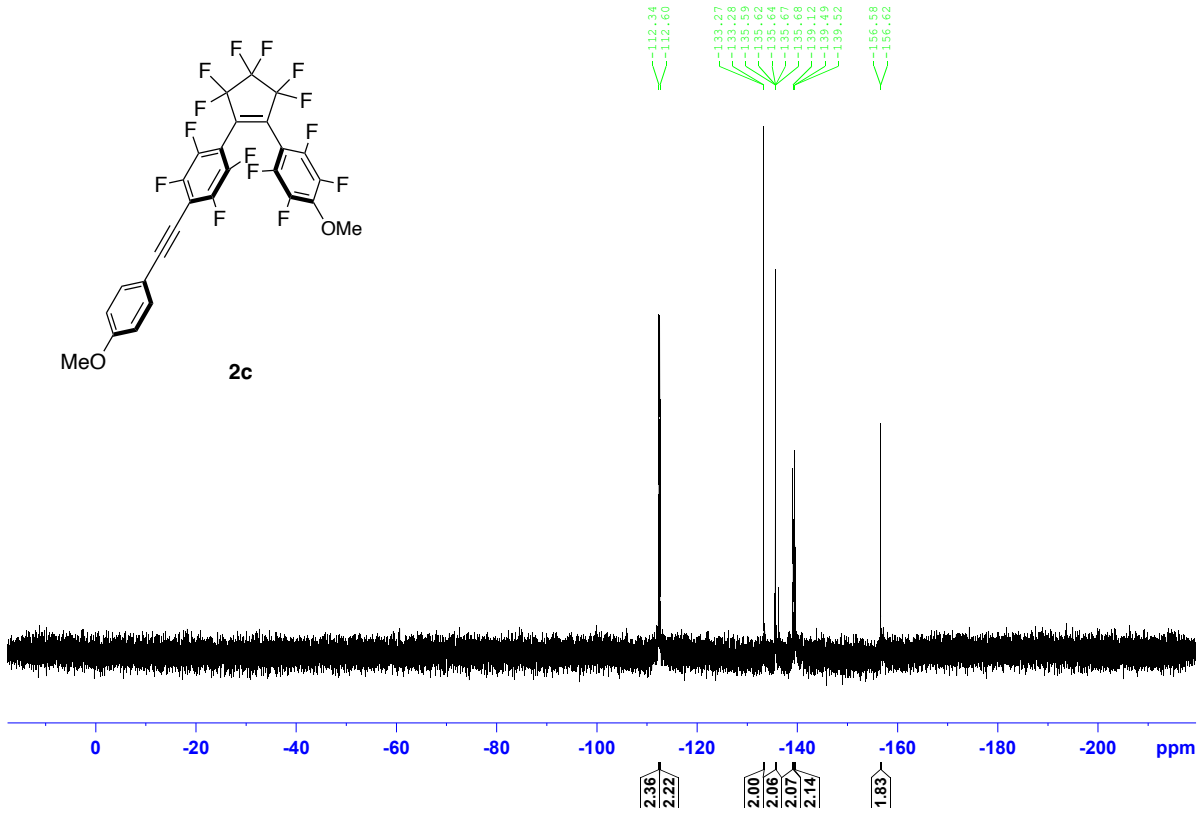


Figure S29. ^{19}F NMR spectrum of **2c** ($CDCl_3$, 376 MHz)

3. DFT calculation

All computations were performed using the Gaussian 16 software package (Revision B.01). Geometry optimizations were carried out using the CAM-B3LYP hybrid functional and the 6-31G(d) basis set with an implicit solvation model (conductor-like polarizable continuum model; CPCM) for CH_2Cl_2. The vertical excitation energies and dipole moments of the optimized structures were calculated using the time-dependent self-consistent field approximation at the same level of theory.

3.1. Optimized geometries

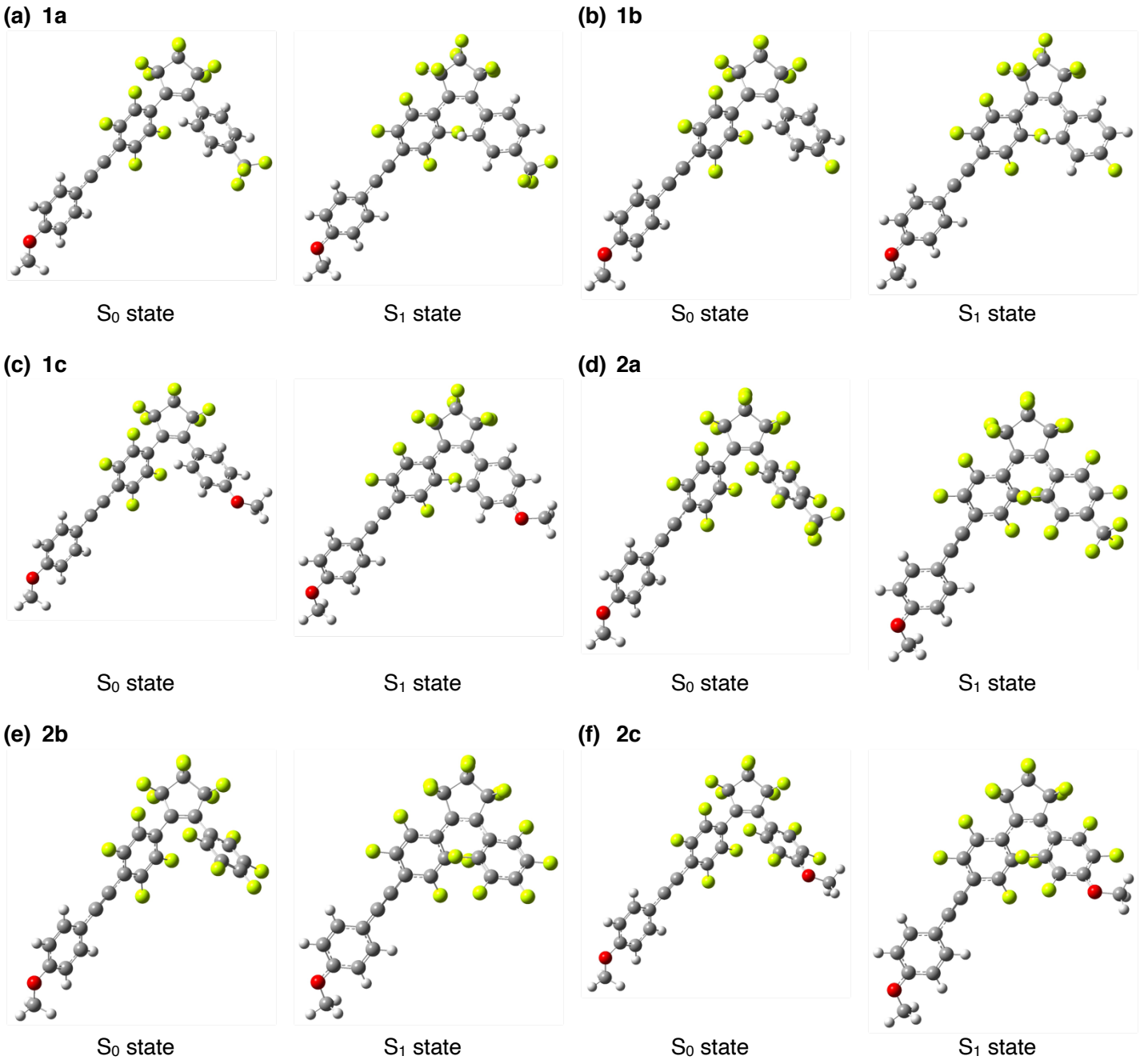
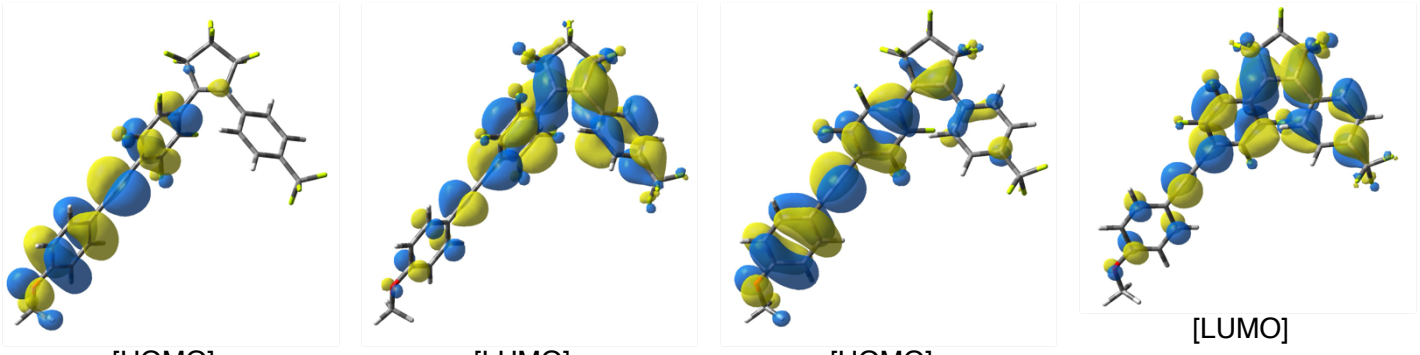


Figure S30. Optimized Geometry of **1a–c** and **2a–c** at both S_0 and S_1 states

3.2. HOMO and LUMO distributions

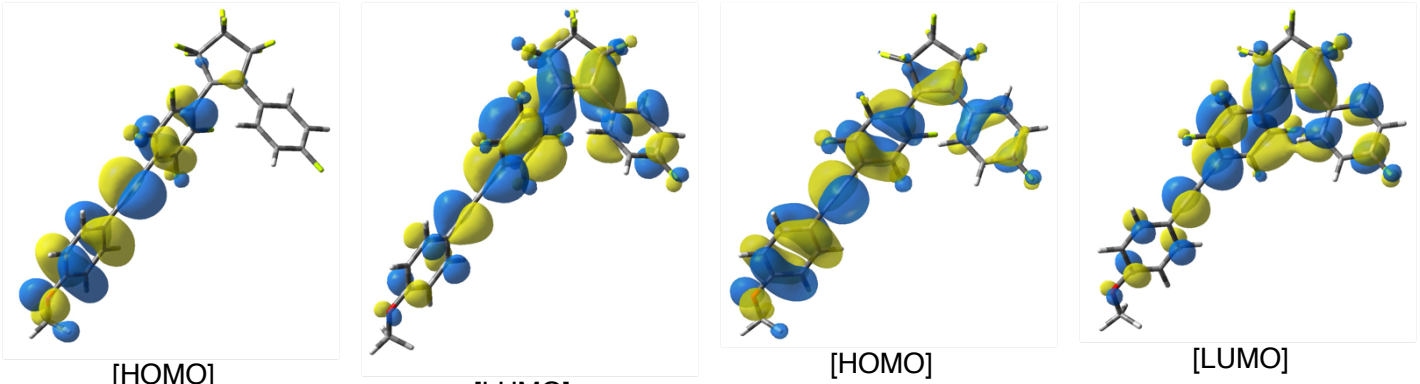
(a) 1a



[HOMO] [LUMO] [HOMO] [LUMO]

S_0 state S_1 state

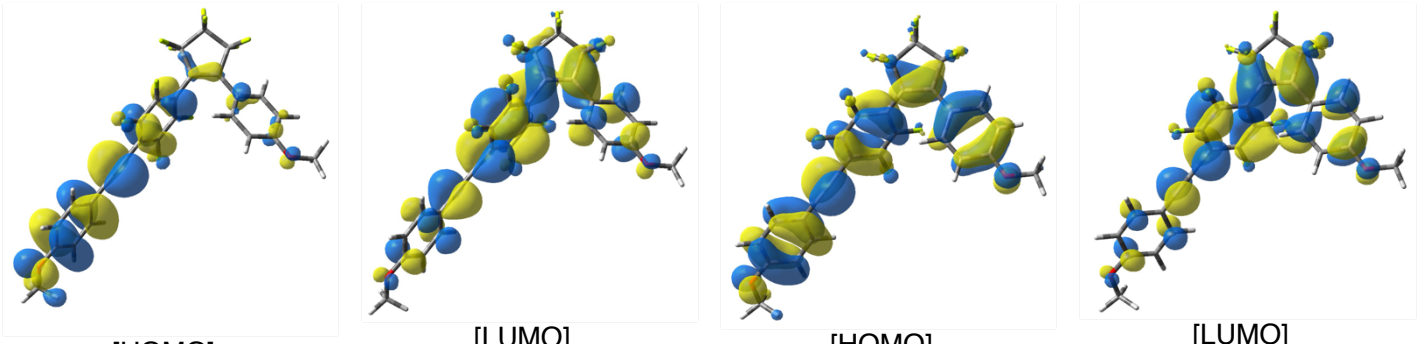
(b) 1b



[HOMO] [LUMO] [HOMO] [LUMO]

S_0 state S_1 state

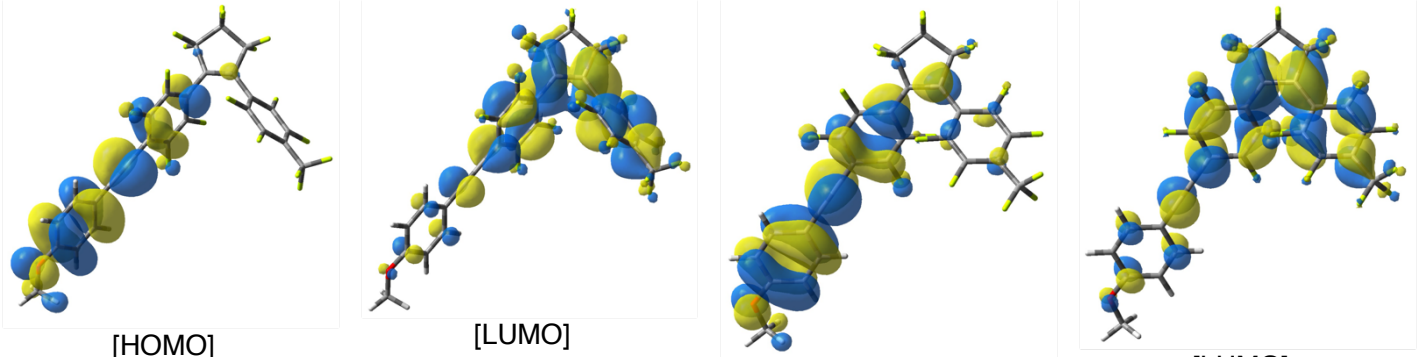
(c) 1c



[HOMO] [LUMO] [HOMO] [LUMO]

S_0 state S_1 state

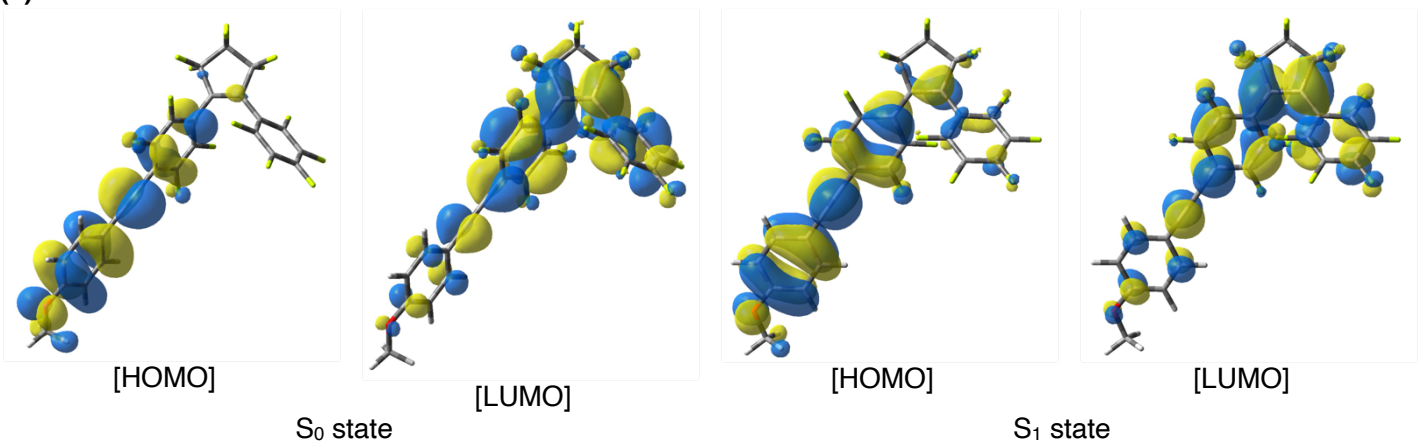
(d) 2a



[HOMO] [LUMO] [HOMO] [LUMO]

S_0 state S_1 state

(e) 2b



(f) 2c

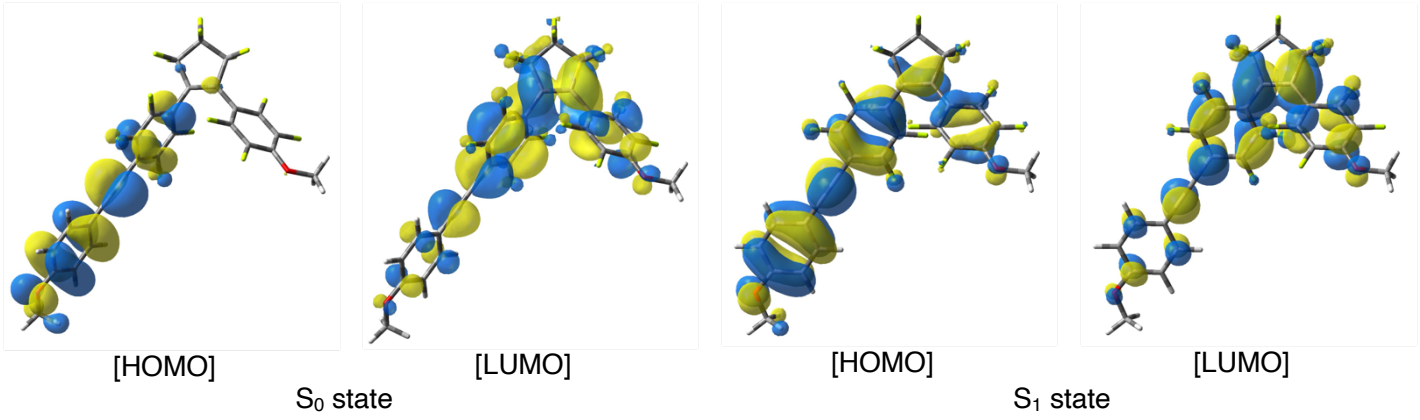


Figure S31. HOMO and LUMO diagrams of **1a–c** and **2a–c** at both S_0 and S_1 states

3.3. Structural and electronic parameters calculated by DFT calculation

Table S1. Structural and electronic parameters for **1a**–**c** and **2a**–**c** at both S_0 and S_1 states

Compound		*Structural parameter*		Electronic parameter	
		C3···C4 distance (pm)	*∠*(C1-C2-C3-C4)(°) /*∠*(C3-C4-C5-C6)(°) [2]	Dipole moment (D)	HOMO/ LUMO [ΔE^{H-L}] (eV) [3]
1a	S_0	134	122/ –39	7.0	–7.55/ –1.72 [5.84]
	S_1	141	154/ –15	10.3	–7.27/ –2.61 [4.66]
1b	S_0	134	121/ –37	7.8	–7.54/ –1.57 [5.97]
	S_1	141	155/ –14	10.6	–7.23/ –2.47 [4.76]
1c	S_0	134	121/ –33	9.4	–7.51/ –1.49 [6.02]
	S_1	142	156/ –11	11.6	–7.13/ –2.38 [4.75]
2a	S_0	134	121/ –52	7.5	–7.58/ –1.97 [5.61]
	S_1	141	160/ –25	12.0	–7.34/ –2.90 [4.44]
2b	S_0	134	120/ –50	7.8	–7.57/ –1.81 [5.76]
	S_1	140	161/ –27	11.8	–7.31/ –2.73 [4.58]
2c	S_0	134	120/ –46	9.4	–7.55/ –1.71 [5.84]
	S_1	141	161/ –25	12.3	–7.26/ –2.63 [4.63]

[1] Calculated using Gaussian 16 with a density functional theory (DFT) method at the CAM-B3LYP/6-311++G(d,p)//CAM-B3LYP/6-31G(d) level of theory with the conductor-like polarizable continuum model (CPCM) for CH_2Cl_2. [2] Dihedral angle defined by indicated four atoms. [3] Orbital energy in eV unit of the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO). ΔE^{H-L}: energy gap (unit: eV) between HOMO and LUMO.

Table S2. Energy (hartree) and dipole moment (debye) of **1a**–**c** and **2a**–**c** at both S_0 and S_1 state.

		E(RCAM-B3LYP) [hartree]	Dipole moment (debye)
1a	S_0	–2408.41830173	X= 6.3207/ Y= 2.7188/ Z= –1.0519/ Tot= 6.9606
	S_1	–2407.66122973	X= 8.3247/ Y= 3.4564/ Z= –0.9792/ Tot= 9.0667
1b	S_0	–2170.59514673	X= –6.6007/ Y= 4.0802/ Z= 0.7062/ Tot= 7.7920
	S_1	–2169.91532131	X= –7.9425/ Y= 4.7701/ Z= 0.4845/ Tot= 9.2775
1c	S_0	–2185.85879664	X= –4.9643/ Y= 7.9213/ Z= 1.3840/ Tot= 9.4502
	S_1	–2185.18007558	X= –4.9604/ Y= 8.7880/ Z= 0.8230/ Tot= 10.1248
2a	S_0	–2805.38177088	X= 7.0162/ Y= 2.2724/ Z= –1.1911/ Tot= 7.4706
	S_1	–2804.48646524	X= 9.6987/ Y= 3.6557/ Z= –0.8706/ Tot= 10.4013
2b	S_0	–2567.55676876	X= 7.0517/ Y= 3.2420/ Z= –1.0945/ Tot= 7.8381
	S_1	–2566.73462626	X= 9.2677/ Y= 4.4754/ Z= –0.5328/ Tot= 10.3055
2c	S_0	–2582.82444154	X= 5.4518/ Y= 7.5100/ Z= –1.8313/ Tot= 9.4592
	S_1	–2582.00394279	X= 6.6352/ Y= 8.4987/ Z= –1.1274/ Tot= 10.8409

3.4. Theoretical transition in S_0 and S_1 states

Table S3. Theoretical transition calculated by TD-DFT calculation using an optimized geometry at the S_0 state.

1a	Excited State 1:	Singlet-A	3.8133 eV	325.14 nm	f=1.3979 <S**2>=0.000
	146(HOMO–3) → 150(LUMO)		0.10178 (2.1%)		
	148(HOMO–1) → 150(LUMO)		0.14274 (4.1%)		
	149(HOMO) → 150(LUMO)		0.58343 (68%)		
	149(HOMO) → 151(LUMO+1)		0.31390 (20%)		
	Excited State 3:	Singlet-A	4.6825 eV	264.78 nm	f=0.2435 <S**2>=0.000
	146(HOMO–3) → 150(LUMO)		-0.29029 (17%)		
	147(HOMO–2) → 150(LUMO)		0.29870 (18%)		
	148(HOMO–1) → 150(LUMO)		-0.13697 (3.7%)		
	148(HOMO–1) → 151(LUMO+1)		0.15345 (4.7%)		
	149(HOMO) → 150(LUMO)		-0.15664 (4.9%)		
	149(HOMO) → 151(LUMO+1)		0.43548 (38%)		
1b	Excited State 1:	Singlet-A	3.8467 eV	322.31 nm	f=1.4426 <S**2>=0.000
	136(HOMO–1) → 138(LUMO)		0.14253 (4.1%)		
	137(HOMO) → 138(LUMO)		0.60647 (74%)		
	137(HOMO) → 139(LUMO+1)		0.26308 (14%)		
	Excited State 2:	Singlet-A	4.6124 eV	268.81 nm	f=0.2537 <S**2>=0.000
	135(HOMO–2) → 138(LUMO)		-0.26809 (14%)		
	136(HOMO–1) → 138(LUMO)		0.50357 (51%)		
	136(HOMO–1) → 139(LUMO+1)		-0.20689 (8.5%)		
	137(HOMO) → 139(LUMO+1)		-0.29406 (17%)		
1c	Excited State 1:	Singlet-A	3.8264 eV	324.03 nm	f=1.4184 <S**2>=0.000
	136(HOMO–5) → 142(LUMO)		0.11213 (2.5%)		
	140(HOMO–1) → 142(LUMO)		0.17457 (6.1%)		
	140(HOMO–1) → 143(LUMO+1)		0.15552 (4.8%)		
	141(HOMO) → 142(LUMO)		0.60596 (73%)		
	141(HOMO) → 143(LUMO+1)		-0.19819 (7.8%)		
	Excited State 2:	Singlet-A	4.2921 eV	288.87 nm	f=0.5598 <S**2>=0.000
	140(HOMO–1) → 142(LUMO)		0.58040 (67%)		
	140(HOMO–1) → 143(LUMO+1)		0.23336 (11%)		
	141(HOMO) → 142(LUMO)		-0.12746 (3.2%)		
	141(HOMO) → 143(LUMO+1)		0.25523 (13%)		
2a	Excited State 1:	Singlet-A	3.7333 eV	332.11 nm	f=1.2878 <S**2>=0.000
	162(HOMO–3) → 166(LUMO)		0.17434 (6.1%)		
	165(HOMO) → 166(LUMO)		0.57560 (66%)		
	165(HOMO) → 167(LUMO+1)		-0.32780 (21%)		
	Excited State 3:	Singlet-A	4.5867 eV	270.31 nm	f=0.2049 <S**2>=0.000
	162(HOMO–3) → 166(LUMO)		0.21106 (8.9%)		
	163(HOMO–2) → 166(LUMO)		0.16729 (5.6%)		
	165(HOMO) → 166(LUMO)		0.27177 (15%)		
	165(HOMO) → 167(LUMO+1)		0.51129 (52%)		
	165(HOMO) → 168(LUMO+2)		-0.17921 (6.4%)		
2b	Excited State 1:	Singlet-A	3.7793 eV	328.06 nm	f=1.3585 <S**2>=0.000
	150(HOMO–3) → 154(LUMO)		0.17082 (5.8%)		
	153(HOMO) → 154(LUMO)		0.59637 (71%)		
	153(HOMO) → 155(LUMO+1)		0.29623 (18%)		
	Excited State 3:	Singlet-A	4.7140 eV	263.01 nm	f=0.1637 <S**2>=0.000
	146(HOMO–7) → 154(LUMO)		0.11411 (2.6%)		
	150(HOMO–3) → 154(LUMO)		-0.25971 (13%)		
	150(HOMO–3) → 155(LUMO+1)		0.12757 (3.2%)		
	153(HOMO) → 154(LUMO)		-0.21708 (9.4%)		

	153(HOMO) → 155(LUMO+1)	0.54160 (59%)				
	153(HOMO) → 158(LUMO+4)	0.11539 (2.7%)				
2c	Excited State 1:	Singlet-A	3.8023 eV	326.08 nm	f=1.3920	<S**2>=0.000
	152(HOMO–5) → 158(LUMO)	0.14344 (4.1%)				
	156(HOMO–1) → 158(LUMO)	0.12845 (3.3%)				
	157(HOMO) → 158(LUMO)	0.59485 (71%)				
	157(HOMO) → 159(LUMO+1)	0.28613 (16%)				
	Excited State 2:	Singlet-A	4.5257 eV	273.96 nm	f=0.3773	<S**2>=0.000
	155(HOMO–2) → 158(LUMO)	0.19492 (7.6%)				
	156(HOMO–1) → 158(LUMO)	0.57108 (65%)				
	156(HOMO–1) → 159(LUMO+1)	-0.19904 (7.9%)				
	157(HOMO) → 159(LUMO+1)	-0.23062 (11%)				

Table S4. Theoretical transition calculated by TD-DFT calculation using an optimized geometry at the S_1 state.

1a	Excited State 1:	Singlet-A	2.7230 eV	455.32 nm	f=1.5977	<S**2>=0.000
	148(HOMO–1) → 150(LUMO)	–0.19397 (7.5%)				
	149(HOMO) → 150(LUMO)	0.65764 (86%)				
	149(HOMO) → 151(LUMO+1)	0.11142 (2.5%)				
	Excited State 2:	Singlet-A	3.8413 eV	322.77 nm	f=0.4768	<S**2>=0.000
	144(HOMO–5) → 150(LUMO)	-0.15806 (5.0%)				
	148(HOMO–1) → 150(LUMO)	-0.59365 (70%)				
	149(HOMO) → 150(LUMO)	-0.12064 (3.0%)				
	149(HOMO) → 151(LUMO+1)	-0.27889 (16%)				
1b	Excited State 1:	Singlet-A	2.7505 eV	450.77 nm	f=1.5727	<S**2>=0.000
	136(HOMO–1) → 138(LUMO)	-0.18895 (7.1%)				
	136(HOMO–1) → 139(LUMO+1)	0.10982 (2.4%)				
	137(HOMO) → 138(LUMO)	0.66023 (87%)				
	Excited State 2:	Singlet-A	3.7742 eV	328.51 nm	f=0.5246	<S**2>=0.000
	133(HOMO–4) → 138(LUMO)	0.11896 (2.8%)				
	136(HOMO–1) → 138(LUMO)	-0.61741 (76%)				
	137(HOMO) → 138(LUMO)	-0.13590 (3.7%)				
	137(HOMO) → 139(LUMO+1)	-0.24687 (12%)				
1c	Excited State 1:	Singlet-A	2.6596 eV	466.18 nm	f=1.4049	<S**2>=0.000
	140(HOMO–1) → 142(LUMO)	-0.17103 (5.8%)				
	140(HOMO–1) → 143(LUMO+1)	0.12119 (2.9%)				
	141(HOMO) → 142(LUMO)	0.66705 (89%)				
	Excited State 2:	Singlet-A	3.6434 eV	340.30 nm	f=0.7990	<S**2>=0.000
	138(HOMO–3) → 142(LUMO)	0.10636 (2.3%)				
	140(HOMO–1) → 142(LUMO)	-0.63003 (79%)				
	141(HOMO) → 142(LUMO)	-0.13545 (3.7%)				
	141(HOMO) → 143(LUMO+1)	-0.21816 (9.5%)				
2a	Excited State 1:	Singlet-A	2.6076 eV	475.47 nm	f=1.5172	<S**2>=0.000
	164(HOMO–1) → 166(LUMO)	0.18271 (6.7%)				
	165(HOMO) → 166(LUMO)	0.66258 (88%)				
	165(HOMO) → 167(LUMO+1)	-0.11711 (2.7%)				
	Excited State 3:	Singlet-A	3.9095 eV	317.14 nm	f=0.3495	<S**2>=0.000
	160(HOMO–5) → 166(LUMO)	0.21057 (8.9%)				
	161(HOMO–4) → 166(LUMO)	-0.11448 (2.6%)				
	164(HOMO–1) → 166(LUMO)	0.58174 (68%)				
	165(HOMO) → 166(LUMO)	-0.11452 (2.6%)				
	165(HOMO) → 167(LUMO+1)	0.24900 (12%)				

2b	Excited State 1:	Singlet-A	2.7057 eV	458.23 nm	f=1.6807	<S**2>=0.000
	152(HOMO–1) → 154(LUMO)		-0.17177 (5.9%)			
	153(HOMO) → 154(LUMO)		0.66323 (88%)			
	153(HOMO) → 155(LUMO+1)		0.11672 (2.7%)			
	Excited State 2:	Singlet-A	3.8939 eV	318.40 nm	f=0.4454	<S**2>=0.000
	148(HOMO–5) → 154(LUMO)		0.14371 (4.1%)			
	151(HOMO–2) → 154(LUMO)		-0.17986 (6.5%)			
	152(HOMO–1) → 154(LUMO)		0.59705 (71%)			
	153(HOMO) → 154(LUMO)		0.10115 (2.0%)			
	153(HOMO) → 155(LUMO+1)		0.22922 (10%)			
2c	Excited State 1:	Singlet-A	2.6955 eV	459.97 nm	f=1.6434	<S**2>=0.000
	156(HOMO–1) → 158(LUMO)		-0.17225 (5.9%)			
	156(HOMO–1) → 159(LUMO+1)		0.10587 (2.2%)			
	157(HOMO) → 158(LUMO)		0.66210 (88%)			
	Excited State 2:	Singlet-A	3.6882 eV	336.16 nm	f=0.5965	<S**2>=0.000
	150(HOMO–7) → 158(LUMO)		0.10320 (2.1%)			
	156(HOMO–1) → 158(LUMO)		0.63786 (81%)			
	157(HOMO) → 158(LUMO)		0.12991 (3.4%)			
	157(HOMO) → 159(LUMO+1)		0.19938 (7.9%)			

3.5. Cartesian coordinate

Table S5. Cartesian coordinate for **1a** at the optimized geometry in S_0 state.

No.	Atom No.	Type	Coordinates (Angstroms) x	y	z
1	9	0	-0.954188	-0.062479	-2.005000
2	9	0	-0.601207	-2.440175	2.055289
3	6	0	-2.300382	2.787906	1.102255
4	9	0	1.679238	0.345509	-1.994743
5	6	0	1.943896	-0.847846	0.025380
6	6	0	-3.999910	3.016835	-0.596078
7	6	0	-2.311306	-1.543800	-0.044343
8	6	0	-0.231534	-0.565487	-1.002090
9	6	0	-3.116923	3.590421	0.312344
10	6	0	5.947417	-0.224644	0.052554
11	6	0	-0.860594	-1.287745	0.009661
12	6	0	-3.305527	-0.642910	-0.081187
13	6	0	-3.232341	0.820841	0.054802
14	9	0	2.030455	-2.051331	2.054292
15	8	0	10.053342	0.356564	0.173257
16	6	0	-2.359123	1.408860	0.974357
17	6	0	8.104223	-0.517753	1.106083
18	1	0	8.725913	-0.902543	1.906931
19	6	0	10.729911	1.079265	-0.843574
20	1	0	10.613355	0.595668	-1.819047
21	1	0	11.782381	1.077802	-0.562180
22	1	0	10.370516	2.111900	-0.902912
23	9	0	-2.303463	-3.844668	0.610631
24	9	0	-2.547469	-3.381703	-1.502486
25	6	0	-2.825400	-2.944480	-0.248144
26	6	0	-4.061714	1.637535	-0.720650
27	6	0	-0.054590	-1.779233	1.033153
28	6	0	3.344636	-0.628359	0.034379
29	6	0	7.937790	0.710926	-0.971876
30	1	0	8.387440	1.271341	-1.781432
31	6	0	6.566603	0.494318	-0.974584
32	1	0	5.965378	0.888937	-1.786593
33	6	0	4.538842	-0.442353	0.041511
34	6	0	1.311367	-1.565389	1.042664
35	6	0	1.133244	-0.349750	-0.997183
36	6	0	8.713832	0.203938	0.072262
37	6	0	6.741180	-0.729220	1.096868
38	1	0	6.274379	-1.288862	1.900179
39	6	0	-4.349911	-2.821686	-0.069027
40	6	0	-4.631160	-1.324984	-0.305791
41	9	0	-4.679956	-3.143316	1.196032
42	9	0	-5.597610	-0.869667	0.516787
43	9	0	-5.030003	-3.608690	-0.914959
44	9	0	-5.069272	-1.148917	-1.581703
45	1	0	-1.739986	0.786655	1.609845
46	1	0	-1.629750	3.237776	1.825127
47	1	0	-4.643543	3.644984	-1.200903
48	1	0	-4.751302	1.194346	-1.428732
49	6	0	-3.012825	5.083308	0.410786
50	9	0	-4.173594	5.687963	0.107865
51	9	0	-2.659846	5.480287	1.644916
52	9	0	-2.086385	5.572569	-0.435090

Table S6. Cartesian coordinate for **1a** at the optimized geometry in S_1 state.

No.	Atom No.	Type	Coordinates (Angstroms) x	y	z
1	9	0	-0.937988	0.390936	-1.612509
2	9	0	-0.32511	-3.027245	1.643548
3	6	0	-2.408899	2.795863	0.935623
4	9	0	1.664109	0.86845	-1.584007
5	6	0	2.074272	-0.824966	0.019466
6	6	0	-4.424271	2.868555	-0.389237
7	6	0	-2.167768	-1.562586	0.050041
8	6	0	-0.172425	-0.303013	-0.765216
9	6	0	-3.451752	3.525132	0.366002
10	6	0	6.00026	-0.105628	0.014114
11	6	0	-0.776655	-1.31501	0.048824
12	6	0	-3.230877	-0.682557	-0.216829
13	6	0	-3.288215	0.743877	-0.040188
14	9	0	2.28618	-2.579468	1.597776
15	8	0	10.076342	0.578961	0.058672
16	6	0	-2.328802	1.431647	0.739917
17	6	0	8.23452	-0.630517	0.792817
18	1	0	8.926411	-1.215566	1.387752
19	6	0	10.689549	1.609879	-0.712395
20	1	0	10.520224	1.449382	-1.780813
21	1	0	11.754161	1.544986	-0.49542
22	1	0	10.312063	2.592875	-0.417311
23	9	0	-2.994176	-3.218043	1.570113
24	9	0	-1.923098	-3.938828	-0.194846
25	6	0	-2.721233	-2.947376	0.263422
26	6	0	-4.349991	1.504424	-0.58579
27	6	0	0.148774	-2.087534	0.819951
28	6	0	3.425851	-0.578718	0.021404
29	6	0	7.891291	1.197261	-0.789677
30	1	0	8.277449	2.000696	-1.403082
31	6	0	6.539802	0.939291	-0.779412
32	1	0	5.86965	1.539608	-1.384216
33	6	0	4.636794	-0.357818	0.018296
34	6	0	1.487838	-1.854435	0.814469
35	6	0	1.166557	-0.066524	-0.774168
36	6	0	8.753414	0.412781	-0.002407
37	6	0	6.889988	-0.88676	0.803948
38	1	0	6.48906	-1.687717	1.414497
39	6	0	-4.050501	-2.934761	-0.510515
40	6	0	-4.472936	-1.455985	-0.528667
41	9	0	-4.980308	-3.725316	0.051469
42	9	0	-5.465793	-1.253482	0.382539
43	9	0	-3.827691	-3.361775	-1.771177
44	9	0	-5.020791	-1.153847	-1.744701
45	1	0	-1.537378	0.877116	1.22898
46	1	0	-1.669348	3.297551	1.549725
47	1	0	-5.243805	3.43112	-0.82242
48	1	0	-5.108368	1.01568	-1.182621
49	6	0	-3.504684	5.01045	0.526993
50	9	0	-4.766913	5.474784	0.509519
51	9	0	-2.943217	5.413423	1.681008
52	9	0	-2.847454	5.649606	-0.463083

Table S7. Cartesian coordinate for **1b** at the optimized geometry in S_0 state.

No.	Atom No.	Type	Coordinates (Angstroms) x	y	z
1	9	0	1.16958	0.651886	1.942677
2	9	0	1.014936	-1.982555	-1.968381
3	6	0	2.251186	3.401602	-1.396628
4	9	0	-1.489001	0.834157	1.925258
5	6	0	-1.654014	-0.493081	-0.020639
6	6	0	4.007994	3.894123	0.202054
7	6	0	2.645668	-0.819383	0.060939
8	6	0	0.491114	0.031438	0.975283
9	6	0	3.046562	4.301753	-0.707291
10	6	0	-5.695879	-0.206371	-0.053973
11	6	0	1.178011	-0.691598	0.002723
12	6	0	3.561304	0.162686	0.017303
13	6	0	3.374199	1.597687	-0.234801
14	9	0	-1.641041	-1.817559	-1.97467
15	8	0	-9.836545	0.027682	-0.170035
16	6	0	2.420937	2.046913	-1.155671
17	6	0	-7.825457	-0.730316	-1.072899
18	1	0	-8.416503	-1.206368	-1.847478
19	6	0	-10.566662	0.740354	0.816335
20	1	0	-10.404845	0.31706	1.813165
21	1	0	-11.61664	0.636496	0.544954
22	1	0	-10.295655	1.801277	0.822077
23	9	0	2.824607	-3.15372	-0.426052
24	9	0	3.031847	-2.522851	1.646871
25	6	0	3.27194	-2.152988	0.362441
26	6	0	4.172273	2.536681	0.43066
27	6	0	0.415115	-1.30962	-0.984252
28	6	0	-3.06848	-0.39263	-0.03348
29	6	0	-7.752688	0.614687	0.937144
30	1	0	-8.243663	1.177789	1.720367
31	6	0	-6.368264	0.512035	0.939529
32	1	0	-5.798372	0.996713	1.724945
33	6	0	-4.273985	-0.306692	-0.042413
34	6	0	-0.964224	-1.213224	-0.998002
35	6	0	-0.887089	0.130381	0.966268
36	6	0	-8.488455	-0.008403	-0.072687
37	6	0	-6.449518	-0.828266	-1.064137
38	1	0	-5.941502	-1.388989	-1.841275
39	6	0	4.780734	-1.920572	0.164751
40	6	0	4.938258	-0.392252	0.283315
41	9	0	5.137268	-2.311595	-1.073591
42	9	0	5.865073	0.073812	-0.578548
43	9	0	5.523666	-2.581735	1.064527
44	9	0	5.362921	-0.083489	1.538861
45	1	0	1.82096	1.332893	-1.707677
46	1	0	1.522572	3.763443	-2.112559
47	1	0	4.612084	4.632512	0.716077
48	1	0	4.91951	2.205665	1.141774
49	9	0	2.885804	5.613695	-0.935322

Table S8. Cartesian coordinate for **1b** at the optimized geometry in S_1 state.

No.	Atom No.	Type	Coordinates (Angstroms) x	y	z
1	9	0	1.16329	1.1456	1.458817
2	9	0	0.863127	-2.592303	-1.47775
3	6	0	2.377453	3.445456	-1.313295
4	9	0	-1.471102	1.364353	1.428761
5	6	0	-1.727107	-0.496509	-0.012889
6	6	0	4.40797	3.825109	-0.034952
7	6	0	2.566657	-0.821021	-0.04985
8	6	0	0.464513	0.309261	0.683496
9	6	0	3.362851	4.290908	-0.823248
10	6	0	-5.710571	-0.1771	-0.005273
11	6	0	1.160994	-0.710291	-0.044772
12	6	0	3.544438	0.178847	0.129365
13	6	0	3.465494	1.579399	-0.175448
14	9	0	-1.777754	-2.39683	-1.427763
15	8	0	-9.841065	0.073563	-0.04678
16	6	0	2.432896	2.103601	-0.992939
17	6	0	-7.883395	-0.996399	-0.700142
18	1	0	-8.512286	-1.701119	-1.232218
19	6	0	-10.548249	1.101828	0.63993
20	1	0	-10.354633	1.057866	1.715645
21	1	0	-11.603183	0.911902	0.449662
22	1	0	-10.276196	2.088139	0.252929
23	9	0	3.551134	-2.508067	-1.437781
24	9	0	2.559067	-3.182063	0.390827
25	6	0	3.253222	-2.157112	-0.155402
26	6	0	4.459422	2.482619	0.280091
27	6	0	0.306773	-1.634047	-0.72922
28	6	0	-3.098789	-0.384689	-0.013606
29	6	0	-7.724377	0.985128	0.710588
30	1	0	-8.188114	1.794685	1.258967
31	6	0	-6.35134	0.869197	0.701685
32	1	0	-5.745382	1.587444	1.242514
33	6	0	-4.324083	-0.287397	-0.009356
34	6	0	-1.048263	-1.530481	-0.722686
35	6	0	-0.891523	0.412994	0.694171
36	6	0	-8.504085	0.05121	0.008405
37	6	0	-6.517743	-1.111003	-0.709364
38	1	0	-6.039701	-1.916812	-1.254807
39	6	0	4.575422	-1.951255	0.60368
40	6	0	4.854375	-0.443156	0.493422
41	9	0	5.57692	-2.69462	0.103336
42	9	0	5.822461	-0.225307	-0.441668
43	9	0	4.39498	-2.289103	1.89798
44	9	0	5.375075	0.012746	1.673744
45	1	0	1.689291	1.435908	-1.409978
46	1	0	1.593974	3.84433	-1.947535
47	1	0	5.160023	4.518939	0.323066
48	1	0	5.264804	2.120868	0.905352
49	9	0	3.311935	5.594348	-1.128913

Table S9. Cartesian coordinate for **1c** at the optimized geometry in S_0 state.

No.	Atom No.	Type	Coordinates (Angstroms) x	y	z
1	9	0	1.069697	0.362726	1.972342
2	9	0	0.816337	-2.161946	-2.005892
3	6	0	2.263726	3.159041	-1.262313
4	9	0	-1.578758	0.653649	1.956308
5	6	0	-1.79343	-0.615038	-0.023519
6	6	0	4.133325	3.523514	0.224475
7	6	0	2.490198	-1.118258	0.053351
8	6	0	0.369282	-0.204663	0.988029
9	6	0	3.147233	4.035026	-0.620205
10	6	0	-5.820108	-0.160128	-0.05736
11	6	0	1.029015	-0.928614	-0.002519
12	6	0	3.449167	-0.174596	0.030012
13	6	0	3.335302	1.268053	-0.196251
14	9	0	-1.830166	-1.889198	-2.010462
15	8	0	-9.946641	0.254673	-0.181577
16	6	0	2.357543	1.799077	-1.051942
17	6	0	-7.96501	-0.560033	-1.100332
18	1	0	-8.571736	-0.985316	-1.892141
19	6	0	-10.650138	0.969431	0.822379
20	1	0	-10.513541	0.509745	1.806793
21	1	0	-11.702062	0.920951	0.543063
22	1	0	-10.331992	2.016502	0.861414
23	9	0	2.562797	-3.448733	-0.478235
24	9	0	2.79248	-2.870192	1.606882
25	6	0	3.052774	-2.483022	0.330234
26	6	0	4.222892	2.152519	0.42273
27	6	0	0.24313	-1.48956	-1.005416
28	6	0	-3.202711	-0.456192	-0.035696
29	6	0	-7.845294	0.71551	0.952143
30	1	0	-8.315837	1.273535	1.751398
31	6	0	-6.466457	0.553892	0.956332
32	1	0	-5.880513	0.988444	1.75908
33	6	0	-4.40359	-0.320287	-0.044735
34	6	0	-1.131287	-1.337397	-1.018028
35	6	0	-1.003671	-0.049104	0.979881
36	6	0	-8.601754	0.157352	-0.080073
37	6	0	-6.594502	-0.716812	-1.089592
38	1	0	-6.106841	-1.27339	-1.882588
39	6	0	4.570265	-2.316784	0.140568
40	6	0	4.797263	-0.800673	0.291365
41	9	0	4.912455	-2.698223	-1.105232
42	9	0	5.752786	-0.364105	-0.555358
43	9	0	5.280713	-3.030517	1.027057
44	9	0	5.229277	-0.538653	1.555367
45	8	0	2.972276	5.347329	-0.886321
46	6	0	3.843429	6.284497	-0.271058
47	1	0	3.523924	7.264966	-0.622227
48	1	0	3.762289	6.24413	0.820035
49	1	0	4.883389	6.112639	-0.567082
50	1	0	1.679542	1.136872	-1.577917
51	1	0	1.516152	3.571825	-1.930496
52	1	0	4.832458	4.177606	0.729256
53	1	0	4.991574	1.771695	1.084847

Table S10. Cartesian coordinate for **1c** at the optimized geometry in S_1 state.

No.	Atom No.	Type	Coordinates (Angstroms) x	y	z
1	9	0	1.076510	0.849657	1.518334
2	9	0	0.618075	-2.769773	-1.546456
3	6	0	2.397364	3.177695	-1.169988
4	9	0	-1.540772	1.189146	1.484013
5	6	0	-1.875303	-0.610541	-0.014612
6	6	0	4.470923	3.424696	0.075777
7	6	0	2.395694	-1.125854	-0.063688
8	6	0	0.347242	0.070993	0.709187
9	6	0	3.433366	3.996472	-0.683021
10	6	0	-5.855055	-0.102077	-0.009362
11	6	0	1.000913	-0.956842	-0.045505
12	6	0	3.420779	-0.168155	0.167921
13	6	0	3.407995	1.227943	-0.106395
14	9	0	-2.009026	-2.457117	-1.491103
15	8	0	-9.976546	0.342834	-0.060641
16	6	0	2.384241	1.836186	-0.892172
17	6	0	-8.060160	-0.793467	-0.736464
18	1	0	-8.715616	-1.453060	-1.294142
19	6	0	-10.629132	1.380682	0.659088
20	1	0	-10.440790	1.293534	1.733699
21	1	0	-11.693121	1.253855	0.464462
22	1	0	-10.307744	2.366023	0.307452
23	9	0	3.349177	-2.783353	-1.511193
24	9	0	2.294331	-3.503337	0.264374
25	6	0	3.033627	-2.478682	-0.220050
26	6	0	4.457332	2.076325	0.346829
27	6	0	0.105395	-1.815135	-0.761573
28	6	0	-3.250298	-0.433879	-0.014992
29	6	0	-7.817863	1.126744	0.730875
30	1	0	-8.243314	1.940937	1.303243
31	6	0	-6.447320	0.945434	0.723371
32	1	0	-5.813482	1.618861	1.289777
33	6	0	-4.463042	-0.279382	-0.011734
34	6	0	-1.245013	-1.646990	-0.753587
35	6	0	-1.005845	0.232650	0.720359
36	6	0	-8.635499	0.255941	-0.000666
37	6	0	-6.697290	-0.971000	-0.742510
38	1	0	-6.256189	-1.781912	-1.311496
39	6	0	4.345147	-2.358570	0.578162
40	6	0	4.692086	-0.860404	0.538615
41	9	0	5.327260	-3.124112	0.072804
42	9	0	5.692163	-0.651007	-0.365570
43	9	0	4.117035	-2.739300	1.853083
44	9	0	5.205528	-0.474111	1.746620
45	8	0	3.351527	5.294370	-0.999340
46	6	0	4.370861	6.184604	-0.555558
47	1	0	4.089139	7.166777	-0.931479
48	1	0	4.419663	6.208849	0.537076
49	1	0	5.344372	5.899131	-0.964818
50	1	0	1.598188	1.220972	-1.311537
51	1	0	1.623989	3.632952	-1.778788
52	1	0	5.280055	4.034871	0.456402
53	1	0	5.255592	1.658016	0.945972

Table S11. Cartesian coordinate for **2a** at the optimized geometry in S_0 state.

No.	Atom No.	Type	Coordinates (Angstroms) x	y	z
1	9	0	-4.087507	0.960188	-1.980122
2	9	0	-1.689153	0.264027	2.023438
3	9	0	-3.852404	3.58927	-1.649296
4	9	0	-1.443959	2.855411	2.353525
5	9	0	-0.716398	-0.377793	-2.096997
6	9	0	-0.306065	-2.624021	2.030113
7	6	0	-2.098269	2.433682	1.275916
8	9	0	1.907301	0.103286	-2.096778
9	6	0	2.200011	-1.022754	-0.04186
10	6	0	-3.316986	2.779127	-0.737933
11	6	0	-2.028694	-1.833121	-0.093897
12	6	0	0.021197	-0.833312	-1.081284
13	6	0	-2.645066	3.316497	0.354789
14	6	0	6.18304	-0.282604	-0.026753
15	6	0	-0.585653	-1.54989	-0.052537
16	6	0	-3.02301	-0.938536	-0.143514
17	6	0	-2.894363	0.520101	0.008375
18	9	0	2.31628	-2.156898	2.025042
19	8	0	10.269729	0.42054	0.080668
20	6	0	-2.225107	1.062717	1.099924
21	6	0	8.345908	-0.485263	1.035243
22	1	0	8.97761	-0.830688	1.846128
23	6	0	10.926433	1.136751	-0.95373
24	1	0	10.824499	0.62596	-1.916888
25	1	0	11.978246	1.172139	-0.672151
26	1	0	10.537839	2.156941	-1.038578
27	9	0	-1.997287	-4.104548	0.644224
28	9	0	-2.343105	-3.720657	-1.472546
29	6	0	-2.556712	-3.240227	-0.224032
30	6	0	-3.44046	1.413597	-0.908934
31	6	0	0.227694	-1.981315	0.99162
32	6	0	3.593496	-0.763085	-0.036754
33	6	0	8.146392	0.683607	-1.07433
34	1	0	8.580639	1.235631	-1.897935
35	6	0	6.782198	0.427138	-1.072108
36	1	0	6.170705	0.782692	-1.894423
37	6	0	4.781684	-0.541551	-0.033078
38	6	0	1.58594	-1.727091	0.996761
39	6	0	1.379537	-0.579188	-1.081319
40	6	0	8.935522	0.226656	-0.016886
41	6	0	6.989684	-0.736455	1.030944
42	1	0	6.538281	-1.288228	1.848357
43	6	0	-4.070514	-3.094131	0.022997
44	6	0	-4.360738	-1.616202	-0.313348
45	9	0	-4.332445	-3.314681	1.324644
46	9	0	-5.304276	-1.096433	0.496284
47	9	0	-4.794513	-3.938505	-0.723374
48	9	0	-4.819146	-1.539991	-1.584316
49	6	0	-2.554061	4.816502	0.464215
50	9	0	-3.778711	5.36048	0.513788
51	9	0	-1.888304	5.214174	1.549577
52	9	0	-1.93256	5.330172	-0.607292

Table S12. Cartesian coordinate for **2a** at the optimized geometry in S_1 state.

No.	Atom No.	Type	Coordinates (Angstroms) x	y	z
1	9	0	-4.607332	0.659011	-1.748029
2	9	0	-1.348676	0.415352	1.699863
3	9	0	-4.843596	3.235297	-1.304266
4	9	0	-1.553575	2.972106	2.081537
5	9	0	-0.645796	0.228076	-1.508075
6	9	0	0.224501	-3.383318	1.483533
7	6	0	-2.315826	2.438583	1.126270
8	9	0	1.917909	0.823515	-1.505414
9	6	0	2.454050	-0.946856	-0.027718
10	6	0	-3.975862	2.543638	-0.560445
11	6	0	-1.758203	-1.878846	0.046772
12	6	0	0.166362	-0.495414	-0.730007
13	6	0	-3.212042	3.211268	0.394994
14	6	0	6.334494	-0.029235	-0.079763
15	6	0	-0.374394	-1.580630	0.031937
16	6	0	-2.844121	-1.036600	-0.248009
17	6	0	-2.950619	0.384521	-0.059654
18	9	0	2.786993	-2.793158	1.415614
19	8	0	10.364674	0.862299	-0.095383
20	6	0	-2.199937	1.079160	0.908938
21	6	0	8.611836	-0.483111	0.612434
22	1	0	9.349755	-1.063827	1.153631
23	6	0	10.909090	1.967255	-0.817226
24	1	0	10.718102	1.861530	-1.888437
25	1	0	11.980586	1.939454	-0.629339
26	1	0	10.493550	2.910154	-0.451983
27	9	0	-2.315846	-3.562349	1.641798
28	9	0	-1.532246	-4.238930	-0.281048
29	6	0	-2.269571	-3.271324	0.313822
30	6	0	-3.854578	1.190977	-0.782292
31	6	0	0.609875	-2.352011	0.728992
32	6	0	3.790716	-0.634200	-0.040876
33	6	0	8.131882	1.416878	-0.852257
34	1	0	8.461093	2.273366	-1.425566
35	6	0	6.797955	1.089191	-0.823910
36	1	0	6.080600	1.687117	-1.374266
37	6	0	4.989470	-0.350932	-0.058500
38	6	0	1.936455	-2.051196	0.708518
39	6	0	1.490689	-0.188511	-0.752342
40	6	0	9.054574	0.632085	-0.133276
41	6	0	7.284558	-0.809285	0.641311
42	1	0	6.940573	-1.664005	1.212164
43	6	0	-3.717798	-3.295068	-0.236621
44	6	0	-4.015113	-1.850030	-0.702030
45	9	0	-4.589709	-3.662154	0.720792
46	9	0	-5.198981	-1.428095	-0.192945
47	9	0	-3.817371	-4.168872	-1.255034
48	9	0	-4.158952	-1.864707	-2.060009
49	6	0	-3.401740	4.688543	0.564411
50	9	0	-4.673744	4.977575	0.888502
51	9	0	-2.618078	5.204970	1.515515
52	9	0	-3.133819	5.343982	-0.578332

Table S13. Cartesian coordinate for **2b** at the optimized geometry in S_0 state.

No.	Atom No.	Type	Coordinates (Angstroms) x	y	z
1	9	0	-4.245444	1.795886	-1.779251
2	9	0	-1.791773	0.675609	2.096755
3	9	0	-3.849776	4.400915	-1.265925
4	9	0	-1.394418	3.280701	2.588432
5	9	0	-0.905235	0.220671	-2.065716
6	9	0	-0.644809	-2.264742	1.93399
7	6	0	-2.08926	2.910634	1.516002
8	9	0	1.744747	0.521498	-2.052453
9	6	0	1.962571	-0.72995	-0.061796
10	6	0	-3.347583	3.481802	-0.445713
11	6	0	-2.312319	-1.245985	-0.134737
12	6	0	-0.199844	-0.337531	-1.079023
13	6	0	-2.616239	3.86977	0.665857
14	6	0	5.986531	-0.25893	-0.030063
15	6	0	-0.85296	-1.064217	-0.086687
16	6	0	-3.245532	-0.285585	-0.118608
17	6	0	-3.026713	1.146727	0.13427
18	9	0	2.003846	-1.97912	1.940823
19	8	0	10.11084	0.171227	0.089651
20	6	0	-2.298589	1.569219	1.246325
21	6	0	8.130898	-0.628092	1.024726
22	1	0	8.737992	-1.03306	1.82681
23	6	0	10.813929	0.864798	-0.929536
24	1	0	10.680051	0.382142	-1.903239
25	1	0	11.86551	0.825651	-0.647565
26	1	0	10.492849	1.909735	-0.992933
27	9	0	-2.423574	-3.556755	0.45983
28	9	0	-2.758463	-3.020347	-1.625316
29	6	0	-2.930996	-2.604242	-0.346935
30	6	0	-3.545517	2.135518	-0.69855
31	6	0	-0.069328	-1.605647	0.928294
32	6	0	3.370634	-0.565429	-0.049863
33	6	0	8.009953	0.599864	-1.056912
34	1	0	8.479929	1.140921	-1.868062
35	6	0	6.631775	0.433931	-1.059147
36	1	0	6.045464	0.84807	-1.872332
37	6	0	4.570975	-0.424265	-0.041292
38	6	0	1.303147	-1.4456	0.940571
39	6	0	1.172812	-0.176762	-1.071917
40	6	0	8.76672	0.067667	-0.011132
41	6	0	6.761042	-0.789457	1.015865
42	1	0	6.273941	-1.32919	1.82074
43	6	0	-4.429447	-2.375862	-0.074909
44	6	0	-4.62359	-0.866364	-0.325992
45	9	0	-4.694728	-2.65043	1.216162
46	9	0	-5.536508	-0.33439	0.510452
47	9	0	-5.213594	-3.12987	-0.856929
48	9	0	-5.071317	-0.691954	-1.59174
49	9	0	-2.421274	5.157867	0.915861

Table S14. Cartesian coordinate for **2b** at the optimized geometry in S_1 state.

No.	Atom No.	Type	Coordinates (Angstroms) x	y	z
1	9	0	-4.714128	1.640941	-1.596078
2	9	0	-1.553734	0.833544	1.854624
3	9	0	-4.711643	4.218970	-0.964883
4	9	0	-1.532650	3.427101	2.412628
5	9	0	-0.870014	0.835700	-1.394178
6	9	0	-0.303415	-3.102094	1.242262
7	6	0	-2.307767	2.978967	1.424792
8	9	0	1.733699	1.197294	-1.378516
9	6	0	2.122259	-0.736128	-0.067091
10	6	0	-3.937946	3.377866	-0.278529
11	6	0	-2.162568	-1.278614	0.010792
12	6	0	-0.122869	-0.021621	-0.688409
13	6	0	-3.120011	3.863182	0.731010
14	6	0	6.070246	-0.169712	-0.090907
15	6	0	-0.756926	-1.115445	-0.012942
16	6	0	-3.164506	-0.316509	-0.198530
17	6	0	-3.128165	1.094956	0.088501
18	9	0	2.296828	-2.736120	1.188573
19	8	0	10.168708	0.348684	-0.074963
20	6	0	-2.323262	1.634683	1.111825
21	6	0	8.300113	-0.888161	0.531275
22	1	0	8.983136	-1.579711	1.010913
23	6	0	10.806987	1.459283	-0.703421
24	1	0	10.604969	1.465355	-1.777991
25	1	0	11.872506	1.321319	-0.530054
26	1	0	10.478091	2.400382	-0.254328
27	9	0	-2.822581	-3.034191	1.487941
28	9	0	-2.204579	-3.611091	-0.525505
29	6	0	-2.806967	-2.630556	0.189143
30	6	0	-3.934244	2.032328	-0.586839
31	6	0	0.163004	-2.036088	0.586942
32	6	0	3.480953	-0.542874	-0.070748
33	6	0	7.991838	1.168001	-0.754686
34	1	0	8.395917	2.038065	-1.255318
35	6	0	6.632765	0.962361	-0.739428
36	1	0	5.971955	1.669843	-1.227182
37	6	0	4.700879	-0.368399	-0.080496
38	6	0	1.510570	-1.854134	0.571457
39	6	0	1.223269	0.165720	-0.706205
40	6	0	8.841058	0.242864	-0.118196
41	6	0	6.948040	-1.093338	0.547072
42	1	0	6.529589	-1.960521	1.044864
43	6	0	-4.274699	-2.460078	-0.279092
44	6	0	-4.415682	-0.975441	-0.681271
45	9	0	-5.130501	-2.746378	0.720611
46	9	0	-5.548433	-0.449502	-0.152672
47	9	0	-4.542787	-3.281964	-1.310212
48	9	0	-4.559179	-0.917392	-2.039738
49	9	0	-3.115109	5.158196	1.029887

Table S15. Cartesian coordinate for **2c** at the optimized geometry in S_0 state.

No.	Atom No.	Type	Coordinates (Angstroms) x	y	z
1	9	0	-4.395936	1.393595	-1.739953
2	9	0	-1.635903	0.549054	1.99602
3	9	0	-4.207332	3.972956	-1.339153
4	9	0	-1.434089	3.162928	2.418949
5	9	0	-0.790648	-0.072845	-2.106574
6	9	0	-0.445618	-2.325078	2.022334
7	6	0	-2.155309	2.729192	1.382738
8	9	0	1.844291	0.336251	-2.105077
9	6	0	2.105439	-0.797323	-0.050028
10	6	0	-3.559056	3.163095	-0.489241
11	6	0	-2.144564	-1.495044	-0.103553
12	6	0	-0.068151	-0.546219	-1.088588
13	6	0	-2.80398	3.668546	0.570923
14	6	0	6.109677	-0.177733	-0.03096
15	6	0	-0.695173	-1.243275	-0.059359
16	6	0	-3.129839	-0.585455	-0.129078
17	6	0	-3.008316	0.85993	0.089689
18	9	0	2.190129	-1.93606	2.016319
19	8	0	10.216488	0.398836	0.086037
20	6	0	-2.257826	1.375301	1.150201
21	6	0	8.261621	-0.437985	1.041074
22	1	0	8.879216	-0.795661	1.857512
23	6	0	10.898669	1.08409	-0.952663
24	1	0	10.784736	0.567105	-1.91119
25	1	0	11.950055	1.090073	-0.667278
26	1	0	10.541993	2.114852	-1.049382
27	9	0	-2.132812	-3.781758	0.583506
28	9	0	-2.475077	-3.353338	-1.525035
29	6	0	-2.68393	-2.891893	-0.26686
30	6	0	-3.656869	1.797938	-0.705406
31	6	0	0.106744	-1.698498	0.983105
32	6	0	3.506382	-0.578433	-0.045096
33	6	0	8.106218	0.717353	-1.079324
34	1	0	8.560331	1.248179	-1.906152
35	6	0	6.734555	0.503537	-1.080069
36	1	0	6.137466	0.870609	-1.907899
37	6	0	4.700726	-0.393353	-0.040011
38	6	0	1.471602	-1.484261	0.988371
39	6	0	1.297303	-0.330359	-1.088417
40	6	0	8.876953	0.245653	-0.014947
41	6	0	6.89816	-0.646892	1.033669
42	1	0	6.426875	-1.177022	1.854195
43	6	0	-4.194373	-2.736608	-0.018077
44	6	0	-4.465733	-1.256439	-0.349687
45	9	0	-4.458546	-2.958315	1.283858
46	9	0	-5.440855	-0.740107	0.423762
47	9	0	-4.92842	-3.573221	-0.764744
48	9	0	-4.873277	-1.177051	-1.639409
49	8	0	-2.613731	4.949441	0.903734
50	6	0	-3.37934	5.992371	0.289149
51	1	0	-3.101145	6.896623	0.82781
52	1	0	-3.124981	6.094853	-0.766412
53	1	0	-4.449313	5.807687	-0.766412

Table S16. Cartesian coordinate for **2c** at the optimized geometry in S_1 state.

No.	Atom No.	Type	Coordinates (Angstroms) x	y	z
1	9	0	-4.703510	1.241255	-1.622093
2	9	0	-1.478831	0.673824	1.813318
3	9	0	-4.862890	3.772696	-1.084217
4	9	0	-1.600566	3.256773	2.313690
5	9	0	-0.782704	0.628578	-1.402397
6	9	0	-0.067169	-3.224299	1.324886
7	6	0	-2.360674	2.754587	1.336803
8	9	0	1.802715	1.090536	-1.390937
9	6	0	2.265405	-0.800802	-0.044112
10	6	0	-4.017660	3.036776	-0.346126
11	6	0	-1.990021	-1.521607	0.034888
12	6	0	-0.005241	-0.186692	-0.678837
13	6	0	-3.224970	3.621374	0.648587
14	6	0	6.194575	-0.078381	-0.086353
15	6	0	-0.598085	-1.295124	0.011804
16	6	0	-3.039807	-0.609129	-0.212929
17	6	0	-3.080422	0.797078	0.053556
18	9	0	2.517314	-2.760035	1.260706
19	8	0	10.274515	0.602131	-0.090733
20	6	0	-2.297243	1.412688	1.057517
21	6	0	8.452755	-0.695042	0.540895
22	1	0	9.161854	-1.351982	1.031533
23	6	0	10.859871	1.726650	-0.741336
24	1	0	10.653597	1.706823	-1.815297
25	1	0	11.931715	1.639670	-0.572270
26	1	0	10.493368	2.661874	-0.308469
27	9	0	-2.609942	-3.263430	1.548733
28	9	0	-1.904673	-3.868758	-0.427353
29	6	0	-2.572930	-2.895877	0.238834
30	6	0	-3.939879	1.686976	-0.622662
31	6	0	0.359068	-2.161672	0.636652
32	6	0	3.619112	-0.554071	-0.053478
33	6	0	8.061886	1.319381	-0.777286
34	1	0	8.428523	2.196150	-1.294868
35	6	0	6.709418	1.059720	-0.754370
36	1	0	6.021475	1.732935	-1.253323
37	6	0	4.828007	-0.332104	-0.068696
38	6	0	1.698238	-1.925628	0.618374
39	6	0	1.333304	0.050987	-0.699421
40	6	0	8.947565	0.442289	-0.128424
41	6	0	7.107370	-0.952768	0.563760
42	1	0	6.725820	-1.827308	1.078392
43	6	0	-4.031212	-2.812632	-0.280652
44	6	0	-4.243615	-1.342722	-0.709577
45	9	0	-4.904158	-3.137526	0.692157
46	9	0	-5.413906	-0.875601	-0.207045
47	9	0	-4.216143	-3.659487	-1.310258
48	9	0	-4.366995	-1.310813	-2.070851
49	8	0	-3.186074	4.900741	1.027281
50	6	0	-4.044852	5.878474	0.429771
51	1	0	-3.812765	6.807010	0.948398
52	1	0	-3.833789	5.983069	-0.635581
53	1	0	-5.093991	5.618998	0.580956
54	9	0	-4.703510	1.241255	-1.622093
55	9	0	-1.478831	0.673824	1.813318
56	9	0	-4.862890	3.772696	-1.084217
57	9	0	-1.600566	3.256773	2.313690
58	9	0	-0.782704	0.628578	-1.402397
59	9	0	-0.067169	-3.224299	1.324886
60	6	0	-2.360674	2.754587	1.336803
61	9	0	1.802715	1.090536	-1.390937
62	6	0	2.265405	-0.800802	-0.044112
63	6	0	-4.017660	3.036776	-0.346126
64	6	0	-1.990021	-1.521607	0.034888
65	6	0	-0.005241	-0.186692	-0.678837

4. Crystal structures

Single crystal X-ray diffractions were recorded on an XtaLAB AFC11 diffractometer (Rigaku, Tokyo, Japan). The reflection data were integrated, scaled, and averaged using CrysAlisPro program (ver. 1.171.39.43a, Rigaku Corporation, Akishima, Japan). Empirical absorption corrections were applied using the SCALE 3 ABSPACK scaleing algorithm (CrysAlisPro). The structures were assigned by a direct method (SHELXT-2018/2) and refined using a full matrix least squares method (SHELXL-2018/3) visualized by Olex2. The crystallographic data were deposited into the Cambridge Crystallographic Data Centre (CCDC) database (CCDC 2104837 for **1c** and 2104836 for **2bB**). These data can be accessible free of charge from the CCDC via www.ccdc.cam.ac.uk/data_request/cis.

Table S17. Crystallographic data

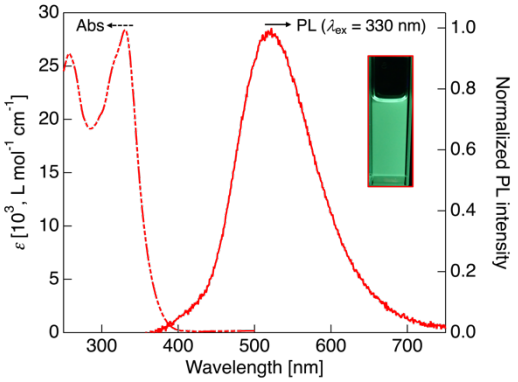
	1c	**2bB**
CCDC No.	2104837	2104836
Empirical formula	$C_{27}H_{14}F_{10}O_2$	$C_{27}H_9F_{15}O$
Formula weight	560.38	634.34
Temperature [K]	298	273
Crystal color / Habit	Colourless / Plate	Colourless / Block
Crystal size [mm]	0.46 x 0.32 x 0.19	0.13 x 0.12 x 0.10
Crystal system	monoclinic	Orthorhombic
Space group	*P 1 2₁/c 1*	*P2₁ 2₁ 2₁*
a [Å]	22.3083(9)	7.5863(7)
b [Å]	7.9227(3)	14.4269(12)
c [Å]	13.7583(5)	23.186(2)
a [°]	90	90
b [°]	99.227(4)	90
g [°]	90	90
V [Å^3]	2400.21(16)	2537.6(4)
Z	4	4
$R\,[F^2 > 2s(F^2)]$ [a]	0.0559	0.0563
$wR\,(F^2)$ [b]	0.1609	0.1283

[a] $R = \Sigma||F_o| - |F_c|| / \Sigma|F_o|$. [b] $wR = \{[\Sigma w(|F_o| - |F_c|)]/\Sigma w|F_o|\}^{1/2}$.

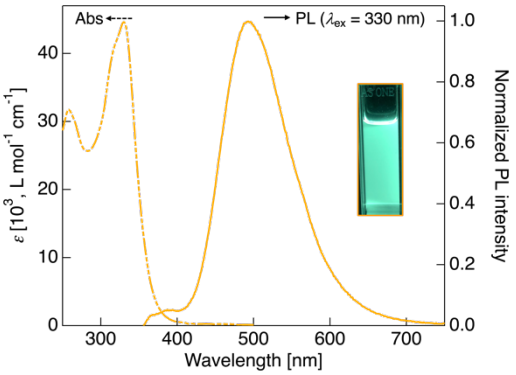
5. Photophysical behavior

5.1. UV-vis and PL spectra of 1a–c and 2a–c in CH_2Cl_2 solution

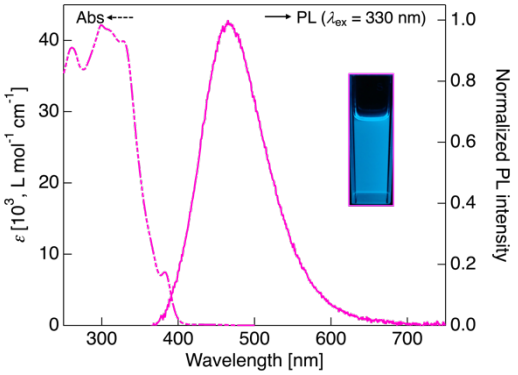
(a) **1a**



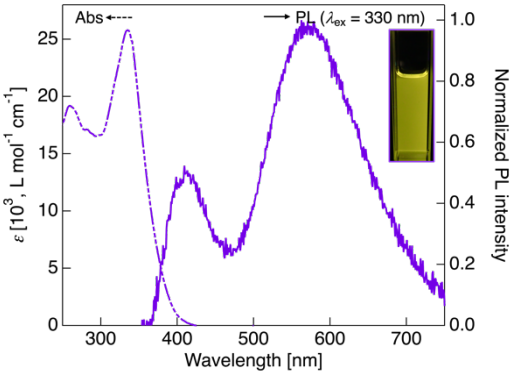
(b) **1b**



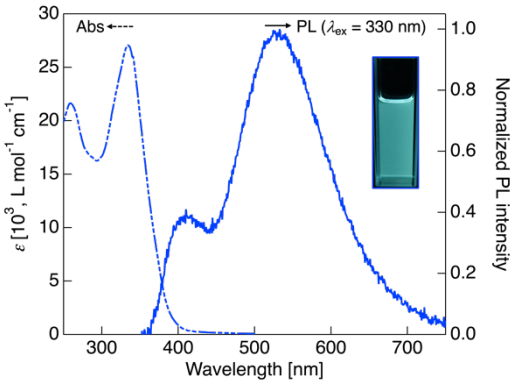
(c) **1c**



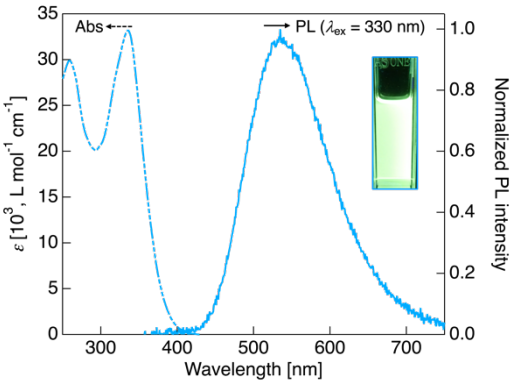
(d) **2a**



(e) **2bA**



(f) **2bB**



(g) **2c**

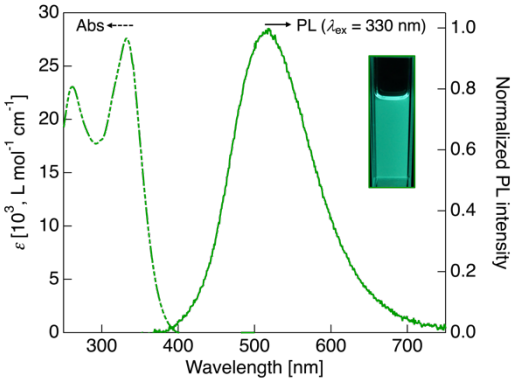


Figure S32. UV-vis absorption and PL spectra of **1a–c** and **2a–c** in CH_2Cl_2 solution. Concentration: 1.0x10^{-5} mol L^{-1} for UV-vis absorption measurement and 1.0x10^{-6} mol L^{-1} for PL measurement.

5.2. Fluorescence decay profiles of 1a–c and 2a–c in CH_2Cl_2 solution

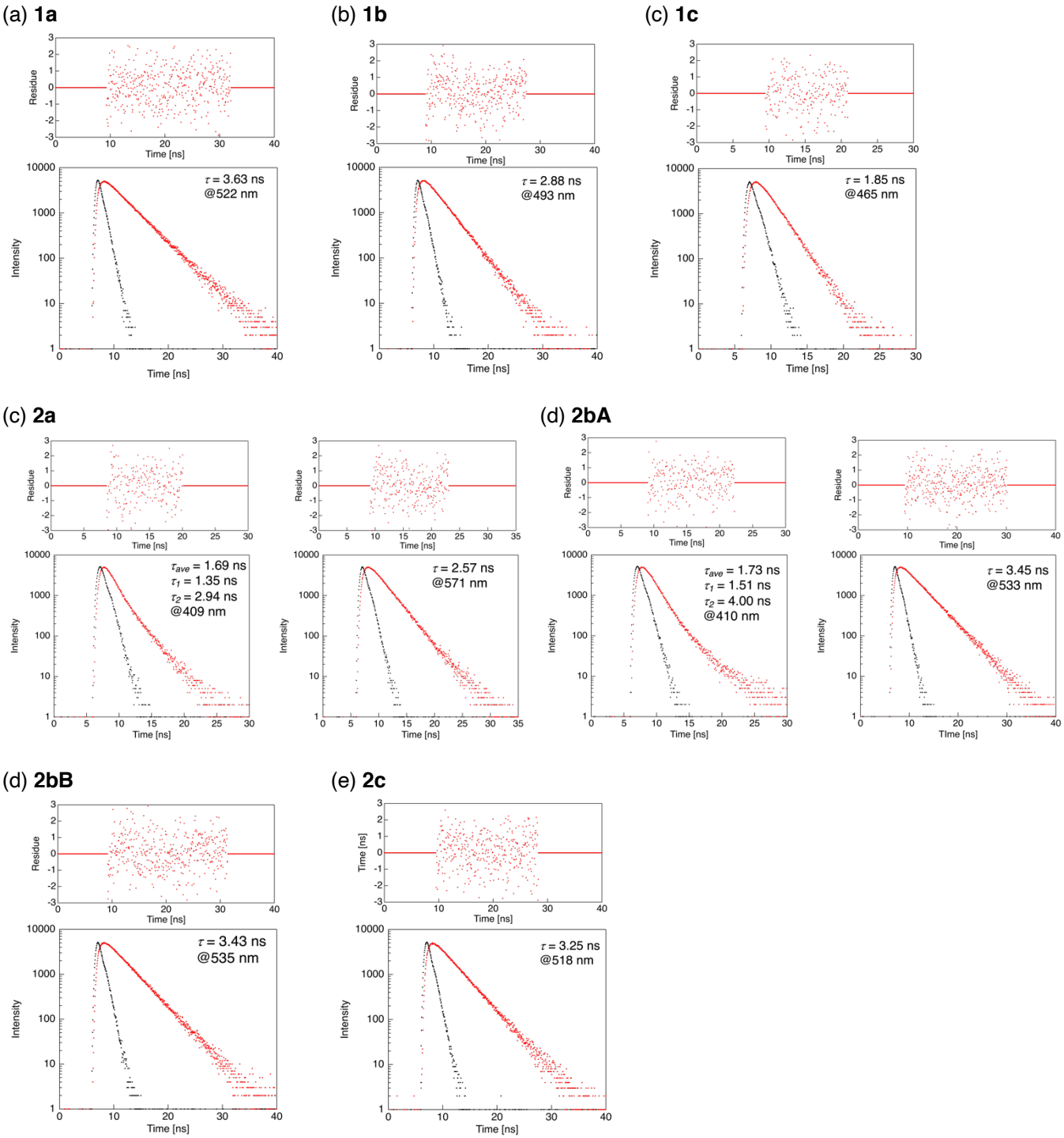


Figure S33. PL lifetime measurement of **1a–c** and **2a–c** in 10^{-6} mol L^{-1} CH_2Cl_2 solution using a Quantaurus-Tau fluorescence lifetime spectrometer (C11367-34)..

Table S18. Average fluorescence lifetime, the radiative and non-radiative rate constant in CH_2Cl_2 solution

Molecule	Φ_{PL} [a]	τ_{ave} [ns]	k_f [10^8, s^{-1}] [b]	k_{nr} [10^8, s^{-1}] [c]
1a	0.99	3.63	2.73	0.02
1b	0.90	2.88	3.12	0.35
1c	0.57	1.85	3.08	2.32
2a	0.35	2.57	1.36	2.53
2bA	0.78	3.45	2.26	0.64
2bB	0.26	3.43	0.76	2.16
2c	0.88	3.25	2.71	0.37

[a] λ_{ex} = 330 nm. [b] Radiative rate constant: $k_f = \Phi_{PL}/\tau_{PL}$. [c] Non-radiative rate constant: $k_{nr} = (1-\Phi_{PL})/\tau_{PL}$.

5.3. UV-vis and PL spectra of 1a in various solution: Solvent effect of photophysical property for 1a

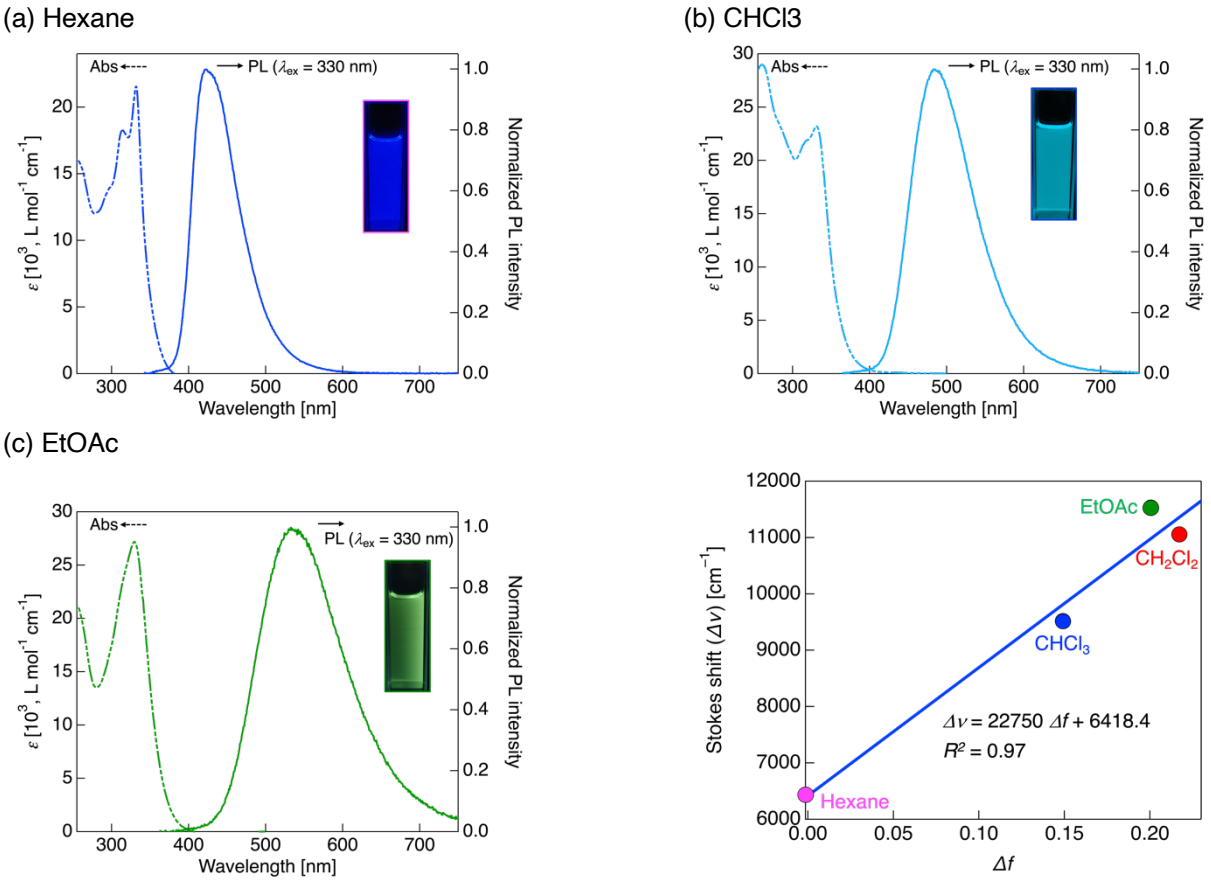


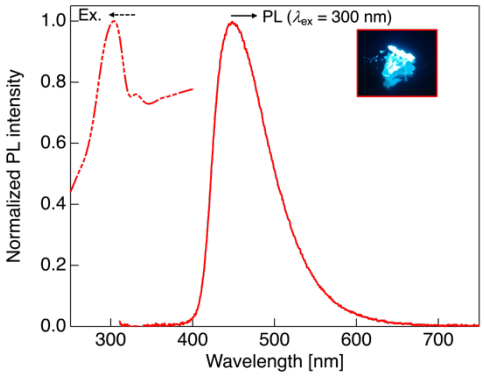
Figure S34. Photophysical properties of **1a** in various solvents: (a) hexane, (b) $CHCl_3$, and (c) EtOAc; (d) Lippert-Mataga prot obtained in the solvent effect for photophysical behavior.

Table S19. Photophysical data of **1a** in various solvents.

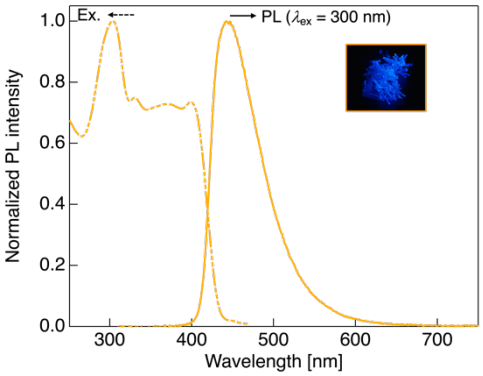
				1a (y=6418.4+22750x) (a=6.48Å) 6.33D		
	Dielectric const.	Refractive index	Δf	ν_{abs} (cm^{-1})	ν_{PL} (cm^{-1})	$\Delta\nu$ (cm^{-1})
Hexane	1.8799	1.3749	-0.0013777	30120	23683	6437
$CHCl_3$	4.806	1.4429	0.14912754	30211	20695	9516
AcOEt	6.02	1.37	0.20050637	30303	18773	11530
CH_2Cl_2	8.93	1.424	0.2171701	30211	19157	11054

5.4. Excitation and PL spectra of 1a–c and 2a–c in crystalline state

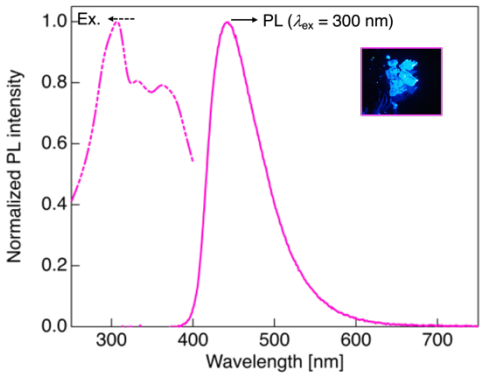
(a) 1a



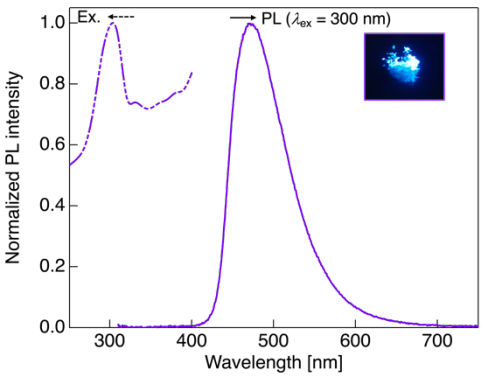
(b) **1b**



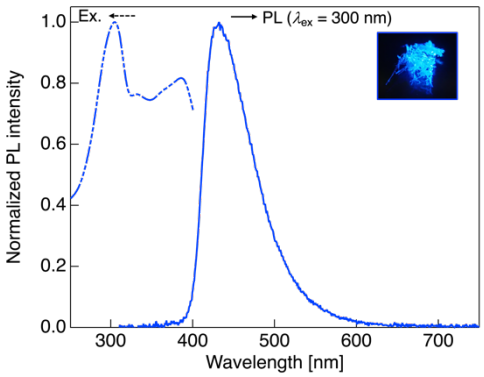
(c) **1c**



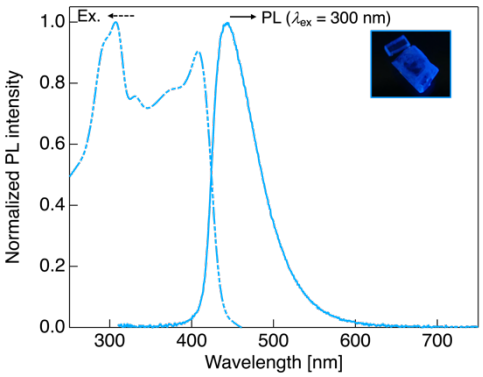
(d) **2a**



(e) **2bA**



(f) **2bB**



(g) **2c**

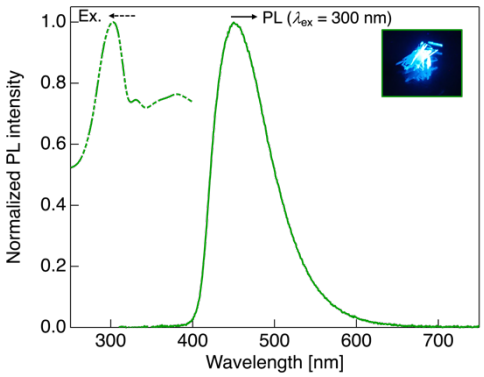


Figure S35. Exicitation and PL spectra of **1a**–**c** and **2a**–**c** in crystalline state.

5.5. Fluorescence decay profiles of 1a–c and 2a–c in crystalline state

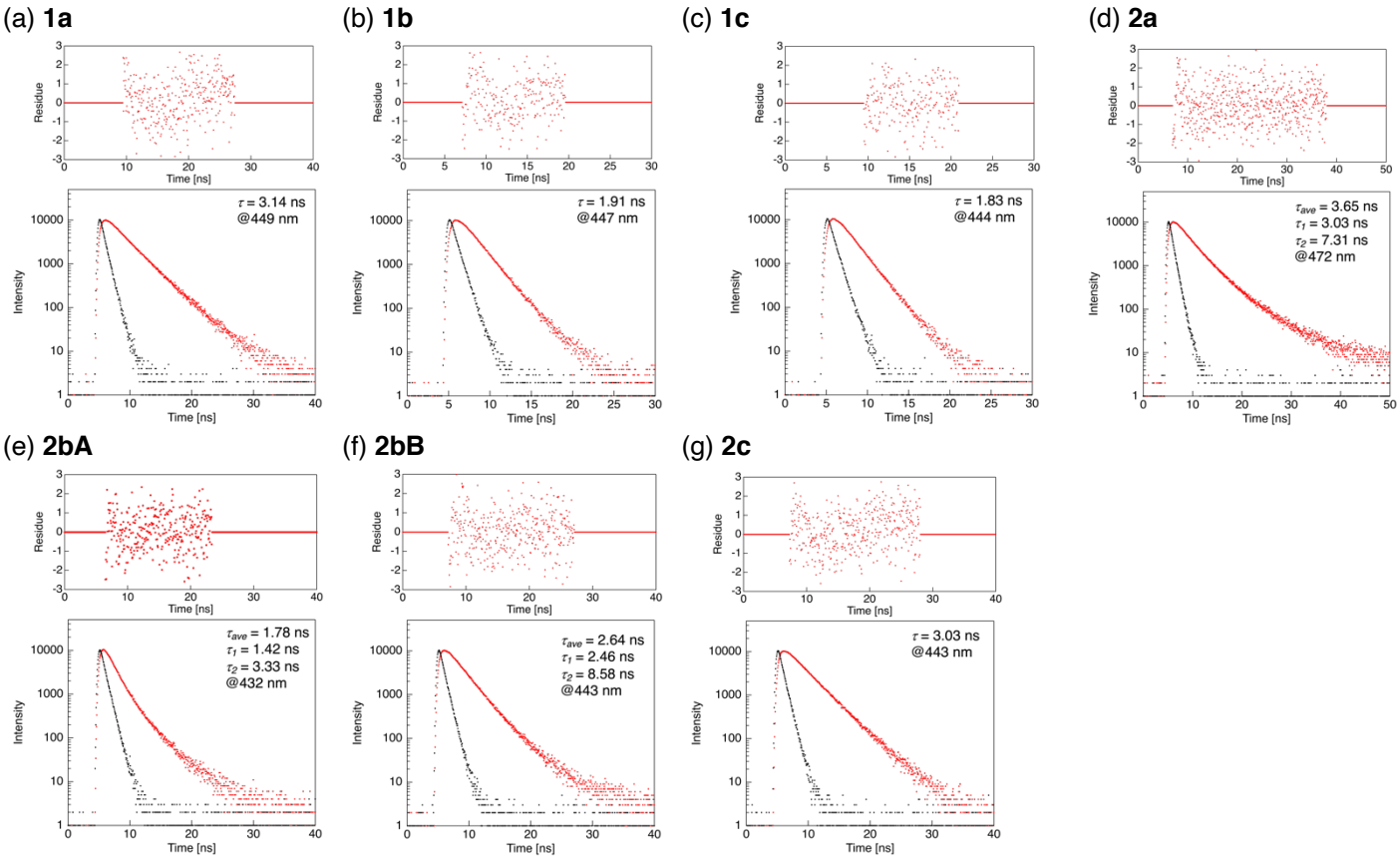


Figure S36. PL lifetime measurement of **1a–c** and **2a–c** in crystal using a Quantaurus-Tau fluorescence lifetime spectrometer (C11367-34).

Table S20. Average fluorescence lifetime, radiative and non-radiative rate constant in crystal

Molecule	Φ_{PL} [a]	τ_{ave} [ns]	k_f [10^8, s^{-1}] [b]	k_{nr} [10^8, s^{-1}] [c]
1a	0.98	3.14	3.12	0.06
1b	1.0	1.91	5.24	0.00
1c	1.0	1.83	5.46	0.00
2a	1.0	3.65	2.74	0.00
2bA	0.52	1.78	2.92	2.70
2bB	0.99	2.64	3.75	0.04
2c	1.0	3.03	3.30	0.00

[a] λ_{ex} = 330 nm. [b] Radiative rate constant: $k_f = \Phi_{PL}/\tau_{PL}$. [c] Non-radiative rate constant: $k_{nr} = (1-\Phi_{PL})/\tau_{PL}$.