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Supporting Information for

Highly Regioselective Palladium-Catalyzed Domino Reaction for Post-Functionalization of BODIPY

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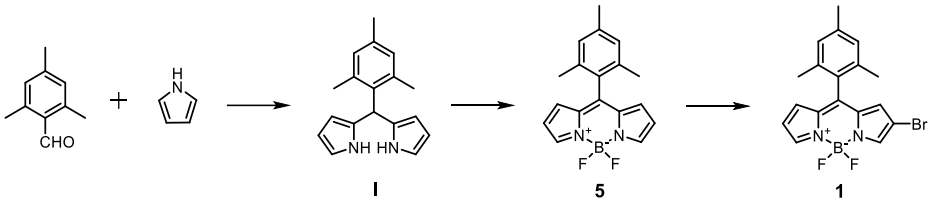
Contents

1 Materials and instrumentations

All reagents were obtained from commercial suppliers and used without further purification unless otherwise indicated. Before doing these air and humidity-sensitive reactions, glassware and solvents are both dehydrated before use. The glassware was dried in an oven at 100 °C and cooled to room temperature under a stream of inert gas, while the solvents (dichloromethane and triethylamine) were distilled over calcium hydride. ^{1}H and ^{13}C NMR spectra were recorded on Bruker DRX400 and Bruker DRX500 spectrometers. HR-MS were recorded on a Bruker Daltonics microTOF-Q II spectrometer. All solvents used for the spectral detection were of spectroscopic grade.

2 Synthesis and characterization



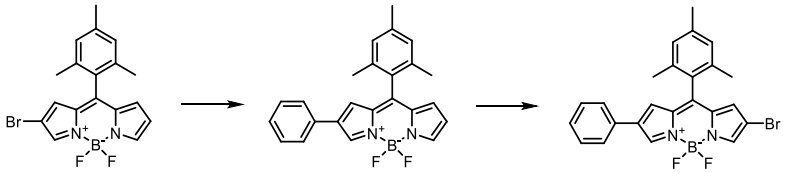
I **5** **1**

Synthesis of **5**

A solution of mesitaldehyde (2.8ml, 19 mmol) in 35 mL pyrrole (494 mmol) with a catalytic amount of trifluoroacetic acid (1.3 mmol) for 1 hour at room temperature under argon. The excess pyrrole is recovered by vacuum distillation. The resulted brownish solid was separated by column chromatography (Hex/DCM = 1/4) to give **I** as a white powder (1.37 g, yield 27%). The precursor **I** was oxidized with one equivalent of DDQ in CH_2Cl_2 for 1 h at room temperature to afford dipyrromethene. Without isolating the dipyrromethene, the reaction mixture was neutralized with triethylamine, after 10 minutes reacted with BF_3▪Et_2O at room temperature for 1 h. The crude reaction mixture was subjected to column chromatographic purification and afforded pure BF_2 complex in 40% yield.

Synthesis of **1**

To a solution of **5** (310 mg, 1.00 mmol) in DMF/CH_2Cl_2 (25 mL/25 mL) was added dropwise a solution of NBS (214 mg, 1.20 mmol) in CH_2Cl_2 (10 mL) at room temperature. The mixture was stirred at room temperature for 30 min. The reaction was monitored by TLC analysis, which finally indicated the presence of **1** as a major product. The resulting mixture was poured into brine and extracted with CH_2Cl_2. The organic layer was dried with Na_2SO_4. After removal of solvents in vacuo, the mixture was purified by silica-gel column chromatography (CH_2Cl_2/hexane = 3:7) to afford **1** (321 mg, 824 μmol) in 82% yield.



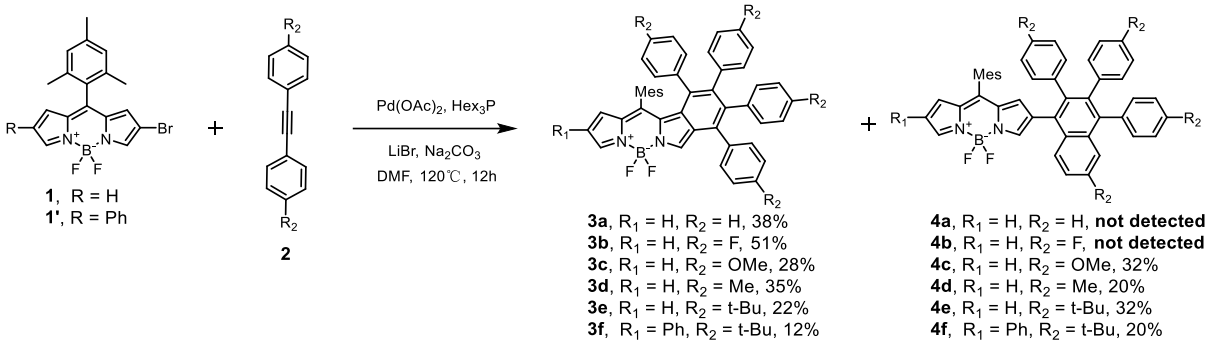
1 **5'** **1'**

Synthesis of **1'**

A mixture of **1** (112 mg, 0.289 mmol), $Pd_2(dba)_3$ (6.6 mg, 0.0072 mmol), DavePhos (11.4 mg, 0.029 mmol), phenylboronic acid (70 mg, 0.574 mmol), and Cs_2CO_3 (312 mg, 0.958 mmol) were placed in a two necked bottle, and 1,4-dioxane/H_2O (2.2 mL, 10:1) was added. Then the reaction mixture was stirred at 80°C, and monitored by TLC analysis. After completion, the resulting mixture was poured into brine and extracted with

EtOAc. The organic layer was dried with Na_2SO_4. After removal of solvents in vacuo, the mixture was purified by silica-gel column chromatography (EtOAc /Hexane = 1:3) to afford **5'** (321 mg, 824 μmol) in 82% yield, which was used in the next step without further purification.

A mixture of **5'** (64 mg, 0.186 mmol) and N-bromosuccinimide (NBS; 43 mg, 0.242 mmol) in anhydrous DMF/CH_2Cl_2 (4 mL, 1:1) was stirred at 70 °C for 30 min, and the solvents were removed under reduced pressure. The residue was purified via flash chromatography (EtOAc/Hexane = 1:10) on silica gel to provide product **1'** (50 mg, 64 %) as a purple solid.



1, R = H
1', R = Ph

2

3a, R_1 = H, R_2 = H, 38%
3b, R_1 = H, R_2 = F, 51%
3c, R_1 = H, R_2 = OMe, 28%
3d, R_1 = H, R_2 = Me, 35%
3e, R_1 = H, R_2 = t-Bu, 22%
3f, R_1 = Ph, R_2 = t-Bu, 12%

4a, R_1 = H, R_2 = H, **not detected**
4b, R_1 = H, R_2 = F, **not detected**
4c, R_1 = H, R_2 = OMe, 32%
4d, R_1 = H, R_2 = Me, 20%
4e, R_1 = H, R_2 = t-Bu, 32%
4f, R_1 = Ph, R_2 = t-Bu, 20%

Synthesis of benzo[*a*]-fused BODIPYs **3a-3f** and naphthyl-BODIPYs **4c-4f**

$Pd(OAc)_2$ (0.03 mmol), LiBr (0.07 mmol) and Na_2CO_3 (0.2 mmol) under nitrogen atmosphere were added to the dry DMF solution (25 mL) of 2-bromo-BODIPY **1/1'** (0.1 mmol) and diphenylacetylene **2** (0.3 mmol). After addition of $PHex_3$ (0.02 mmol) in DMF (1 mL), the reaction mixture was stirred at 120°C for 24 hours. After cooling down, the volatiles were evaporated under reduced pressure. The residue was diluted in CH_2Cl_2, washed with H_2O, dried over $MgSO_4$, filtered and concentrated. The crude material was purified by chromatography over silica gel (dichloromethane/ petroleum ether 2:5) to provide compound **3a** as a golden solid in 38% yield. ^{1}H NMR (400 MHz, CD_2Cl_2) δ 8.49 (s, 1H), 7.42 (s, 1H), 7.30 – 7.24 (m, 5H), 6.88 – 6.85 (m, 3H), 6.81 (dt, J = 8.6, 2.9 Hz, 2H), 6.76 – 6.70 (m, 4H), 6.67 – 6.63 (m, 2H), 6.53 – 6.47 (m, 4H), 6.38 (s, 2H), 6.16 (dd, J = 3.8, 2.3 Hz, 1H), 5.72 (d, J = 3.0 Hz, 1H), 2.14 (s, 3H), 1.82 (s, 6H). ^{13}C NMR (100 MHz, CD_2Cl_2) δ 148.98, 147.96, 141.84, 140.26, 139.51, 139.01, 138.16, 137.59, 137.01, 136.36, 135.28, 134.20, 132.46, 132.20, 132.03, 131.58, 130.96, 130.91, 129.83, 128.93, 128.32, 127.81, 127.10, 126.82, 126.56, 126.17, 125.97, 125.64, 124.98, 21.05, 20.80. UV/Vis (CH_2Cl_2): λ_{max} (ε)= 550 nm (61 060 dm^3 mol^{-1} cm^{-1}); HR-MS: calcd for $C_{46}H_{35}BF_2N_2Na$ $[M + Na]^+$: 687.2761; found 687.2762.

Compounds **3b** was obtained as orange red powder by following a procedure similar to that of **3a** in 51% yield.

For **3b**: ^{1}H NMR (500 MHz, CD_2Cl_2) δ 8.49 (s, 1H), 7.47 (s, 1H), 7.23 – 7.19 (m, 2H), 7.02 (t, J = 8.7 Hz, 2H), 6.76 – 6.72 (m, 2H), 6.63 (t, J = 8.8 Hz, 2H), 6.53 – 6.45 (m, 8H), 6.38 (t, J = 8.8 Hz, 2H), 6.19 (dd, J = 3.7, 2.2 Hz, 1H), 5.74 (d, J = 3.6 Hz, 1H), 2.19 (s, 3H), 1.85 (s, 6H). ^{13}C NMR (100 MHz, CD_2Cl_2) δ 163.03, 161.87, 161.57, 160.58, 159.44, 159.14, 147.32, 146.20, 141.64,138.69, 137.96, 136.66, 135.68, 135.38, 135.12, 134.60, 134.38, 134.14, 133.52, 132.55, 132.28, 132.20, 131.82, 131.74, 131.66, 131.58, 130.86, 130.66, 130.58, 127.84, 125.07, 114.89, 114.67, 114.33, 113.76, 113.55, 113.29, 113.23, 113.07, 113.01, 20.24, 19.99. UV/Vis (CH_2Cl_2): λ_{max} (ε)= 552 nm (59 390 dm^3 mol^{-1} cm^{-1}); HR-MS: calcd for $C_{46}H_{31}BF_6N_2Na$ $[M + Na]^+$: 759.2384; found 759.2397.

When there was an electron-donating group (-OMe, -Me, -t-Bu) on the benzene ring, the reaction not only

generated benzo[*a*]-fused BODIPYs **3c**-**3f**, but also gave a few amount of the corresponding naphthalene-BODIPY dyes **4c**-**4f**.

For **3c** (red powder, 28%): ^{1}H NMR (400 MHz, CD_2Cl_2) δ 8.49 (s, 1H), 7.42 (s, 1H), 7.30 – 7.24 (m, 5H), 6.88 – 6.85 (m, 3H), 6.81 (dt, J = 8.6, 2.9 Hz, 2H), 6.76 – 6.70 (m, 4H), 6.67 – 6.63 (m, 2H), 6.53 – 6.47 (m, 4H), 6.38 (s, 2H), 6.16 (dd, J = 3.8, 2.3 Hz, 1H), 5.72 (d, J = 3.0 Hz, 1H), 2.14 (s, 3H), 1.82 (s, 6H). ^{13}C NMR (100 MHz, CD_2Cl_2) δ 158.32, 157.86, 157.81, 157.58, 149.63, 148.41, 141.17, 140.98, 140.60, 138.17, 138.07, 137.08, 136.51, 135.83, 135.30, 134.13, 133.56, 132.77, 132.64, 132.54, 132.13, 131.99, 131.88, 130.85, 130.10, 128.50, 124.46, 114.39, 113.92, 112.63, 112.47, 112.20, 111.97, 55.62, 55.26, 21.18, 20.98. UV/Vis (CH_2Cl_2): λ_{max} (ε)= 556 nm (45 270 dm^3 mol^{-1} cm^{-1}); HR-MS: calcd for $C_{50}H_{43}BF_2N_2NaO_4$ $[M + Na]^+$: 807.3185; found 807.3177.

For **4c** (red powder, 32%): ^{1}H NMR (500 MHz, CD_2Cl_2) δ 7.83 (d, *J* = 9.1 Hz, 2H), 7.69 (s, 1H), 7.11 (dd, *J* = 9.2, 2.6 Hz, 1H), 7.07 – 7.04 (m, 2H), 6.92 (s, 2H), 6.87 (d, *J* = 2.6 Hz, 1H), 6.80 – 6.72 (m, 6H), 6.62 (d, *J* = 4.0 Hz, 1H), 6.52 – 6.43 (m, 5H), 6.35 (s, 1H), 3.77 (s, 3H), 3.67 (d, *J* = 5.9 Hz, 6H), 3.62 (s, 3H), 2.32 (s, 3H), 2.00 (s, 6H). ^{13}C NMR (126 MHz, CD_2Cl_2) δ 158.46, 158.01, 157.49, 147.37, 146.99, 143.51, 139.96, 139.21, 138.26, 138.03, 136.61, 135.62, 134.31, 133.67, 133.49, 132.49, 131.68, 130.03, 129.77, 128.35, 128.14, 127.43, 118.47, 113.43, 112.74, 112.37, 106.35, 55.43, 55.31, 55.20, 21.25, 19.90. UV/Vis (CH_2Cl_2): λ_{max} (ε)= 526 nm (39 610 dm^3 mol^{-1} cm^{-1}); HR-MS: calcd for $C_{50}H_{43}BF_2N_2NaO_4$ $[M + Na]^+$: 807.3176; found 807.3179.

For **3d** (orange red powder, 35%): ^{1}H NMR (400 MHz, CD_2Cl_2) δ 8.44 (s, 1H), 7.39 – 7.38 (t, 1H), 7.10 (s, 4H), 6.69 (s, 4H), 6.57 (d, *J* = 7.8 Hz, 2H), 6.42 (m, 6H), 6.34 (d, *J* = 8.0 Hz, 2H), 6.13 (dd, *J* = 3.8, 2.3 Hz, 1H), 5.65 (d, *J* = 2.9 Hz, 1H), 2.33 (s, 3H), 2.17 (s, 3H), 2.13 (s, 3H), 2.10 (s, 3H), 2.05 (s, 3H), 1.80 (s, 6H). ^{13}C NMR (125 MHz, CD_2Cl_2) δ 149.57, 148.21, 141.11, 140.50, 138.26, 138.16, 137.57, 137.28, 137.20, 136.72, 136.41, 136.16, 135.64, 135.40, 135.14, 134.82, 134.09, 133.56, 132.55, 132.46, 131.41, 130.80, 130.78, 129.60, 129.00, 128.30, 127.80, 127.48, 127.24, 124.50, 114.36, 30.11, 21.32, 21.30, 21.19, 21.14, 21.07, 20.92. UV/Vis (CH_2Cl_2): λ_{max} (ε)= 552 nm (47 530 dm^3 mol^{-1} cm^{-1}); HR-MS: calcd for $C_{50}H_{43}BF_2N_2$ $[M + Na]^+$: 743.3380; found 743.3361.

For **4d** (orange red powder, 20%): ^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.81 – 7.78 (m, 2H), 7.69 (s, 1H), 7.31 – 7.25 (m, 2H), 7.07 – 7.00 (m, 4H), 6.92 (s, 2H), 6.79 – 6.69 (m, 8H), 6.61 (d, *J* = 4.1 Hz, 1H), 6.46 (dd, *J* = 4.0, 1.7 Hz, 1H), 6.35 (s, 1H), 2.36 (s, 3H), 2.32 (d, *J* = 2.5 Hz, 6H), 2.16 (s, 3H), 2.10 (s, 3H), 1.99 (s, 6H). . ^{13}C NMR (125 MHz, CD_2Cl_2) δ 147.30, 147.13, 143.32, 139.45, 139.27, 139.20, 138.85, 138.18, 138.14, 137.05, 136.60, 136.27, 136.09 135.75, 135.07, 132.94, 131.83, 131.44, 131.34, 130.27, 129.95, 129.84, 129.64, 128.72, 128.55, 128.32, 127.94, 127.60, 126.44, 126.32, 118.40, 32.01, 23.07, 21.91, 21.35, 21.25, 21.19, 21.14, 19.85, 14.30. UV/Vis (CH_2Cl_2): λ_{max} (ε)= 524 nm (37 390 dm^3 mol^{-1} cm^{-1}); HR-MS: calcd for $C_{50}H_{43}BF_2N_2$ $[M + Na]^+$: 743.3380; found 743.3364.

For **3e** (orange red powder, 22%): ^{1}H NMR (500 MHz, CD_2Cl_2) δ 8.51 (s, 1H), 7.40 (t, 1H), 7.30 – 7.27 (m, 2H), 7.16 – 7.13 (m, 2H), 6.89 – 6.87 (m, 2H), 6.71 – 6.69 (m, 4H), 6.65 – 6.62 (m, 2H), 6.38 (s, 2H), 6.31 – 6.27 (m, 4H), 6.16 – 6.15 (m, 1H), 5.74 – 5.73 (m, 1H), 2.13 (s, 3H), 1.80 (s, 6H), 1.29 (s, 9H), 1.19 (s, 9H), 1.09 (s, 9H), 1.06 (s, 9H). ^{13}C NMR (125 MHz, CD_2Cl_2) δ 150.69, 149.63, 149.07, 148.75, 148.33, 147.98, 140.76, 140.58, 138.20, 137.80, 137.27, 137.24, 136.75, 136.36, 135.33, 134.77, 133.91, 133.53, 132.63, 132.34, 132.20, 131.34, 130.63, 130.35, 130.04, 129.37, 128.62, 125.16, 124.26, 123.84, 123.44, 123.18, 114.35, 34.82, 34.44, 34.34, 34.30, 31.46,

31.40, 31.31, 31.24, 30.10, 21.23, 20.88, 1.18. UV/Vis (CH_2Cl_2): λ_{max} (ε)= 553 nm (49 850 $dm^3\,mol^{-1}\,cm^{-1}$); HR-MS: calcd for $C_{62}H_{67}BF_2N_2$ $[M + Na]^+$: 911.5258; found 911.5249.

For **4e** (orange red powder, 32%): ^{1}H NMR (500 MHz, CD_2Cl_2) δ 7.83 – 7.80 (t, 2H), 7.65 (s, 1H), 7.54 (dd, *J* = 8.9, 2.0 Hz, 1H), 7.50 (d, *J* = 1.9 Hz, 1H), 7.25 (d, *J* = 8.4 Hz, 2H), 7.07 (d, *J* = 8.2 Hz, 2H), 6.97 (d, *J* = 8.3 Hz, 2H), 6.92 (s, 2H), 6.86 (d, *J* = 8.3 Hz, 2H), 6.75 (d, *J* = 7.9 Hz, 2H), 6.69 (d, *J* = 8.3 Hz, 2H), 6.60 (d, *J* = 4.0 Hz, 1H), 6.50 (s, 1H), 6.45 (dd, *J* = 4.0, 1.6 Hz, 1H), 2.32 (s, 3H), 2.01 (s, 6H), 1.28 (s, 9H), 1.23 (s, 9H), 1.15 (s, 9H), 1.10 (s, 9H). ^{13}C NMR (125 MHz, CD_2Cl_2) δ 149.60, 149.03, 148.87, 148.36, 147.41, 147.15, 143.16, 139.80, 139.49, 139.37, 139.20, 138.18, 137.97, 137.03, 136.63, 135.71, 135.41, 132.79, 132.60, 131.86, 131.33, 131.21, 131.11, 130.20, 130.03, 129.50, 129.19, 128.40, 126.06, 125.30, 124.57, 124.04, 123.57, 122.72, 118.27, 35.12. 34.71, 34.49, 34.38, 31.43, 31.34, 31.30, 31.10, 30.10, 21.25, 20.08. UV/Vis (CH_2Cl_2): λ_{max} (ε)= 523 nm (40 760 $dm^3\,mol^{-1}\,cm^{-1}$); HR-MS: calcd for $C_{62}H_{67}BF_2N_2$ $[M + Na]^+$: 911.5258; found 911.5243.

For **3f** (purple powder, 12%): ^{1}H NMR (500 MHz, CD2Cl2) δ 8.55 (s, 1H), 7.74 (s, 1H), 7.36 (d, J = 7.3 Hz, 2H), 7.28 (m, 4H), 7.14 (dd, J = 15.5, 7.9 Hz, 3H), 6.88 (d, J = 8.4 Hz, 2H), 6.70 (dd, J = 8.3, 4.1 Hz, 4H), 6.65 (d, J = 8.3 Hz, 2H), 6.41 (s, 2H), 6.30 (d, J = 8.0 Hz, 4H), 5.98 (s, 1H), 2.16 (s, 3H), 1.84 (s, 6H), 1.30 (s, 9H), 1.20 (s, 9H), 1.09 (s, 9H), 1.07 (s, 9H). ^{13}C NMR (126 MHz, CD_2Cl_2) δ 150.74, 150.12, 149.03, 148.37, 148.03, 140.73, 140.46, 138.36, 137.93, 137.30, 136.70, 136.3, 134.67, 132.34, 132.00, 131.33, 130.64, 130.34, 130.04, 129.36, 128.96, 128.76, 126.55, 125.25, 123.86, 123.46, 123.20, 120.00, 34.82, 34.45, 34.35, 34.31, 31.47, 31.40, 31.32, 31.24, 21.29, 20.94. UV/Vis (CH_2Cl_2): λ_{max} (ε)= 582 nm (47 180 $dm^3\,mol^{-1}\,cm^{-1}$); HR-MS: calcd for $C_{68}H_{71}BF_2N_2$ $[M + H]^+$: 965.5751; found 965.5726.

For **4f** (golden solid, 20%): ^{1}H NMR (500 MHz, CD_2Cl_2) δ 8.16 (s, 1H), 7.84 (d, J = 8.9 Hz, 1H), 7.66 (s, 1H), 7.55 (dd, J = 8.9, 2.0 Hz, 1H), 7.50 (m, 3H), 7.35 (t, J = 7.7 Hz, 2H), 7.26 (d, J = 8.5 Hz, 3H), 7.08 (s, 2H), 6.99 – 6.95 (m, 4H), 6.86 (d, J = 8.5 Hz, 2H), 6.81 (s, 1H), 6.76 (d, J = 8.1 Hz, 2H), 6.70 (d, J = 8.4 Hz, 2H), 6.52 (s, 1H), 2.34 (s, 3H), 2.06 (s, 6H), 1.28 (s, 9H), 1.24 (s, 9H), 1.16 (s, 9H), 1.10 (s, 9H). ^{13}C NMR (126 MHz, CD_2Cl_2) δ 149.61, 149.07, 148.89, 148.38, 147.64, 146.78, 140.86, 139.80, 139.49, 139.41, 139.28, 138.17, 137.96, 137.02, 136.71, 135.96, 133.19, 132.61, 131.80, 131.34, 131.21, 131.13, 130.19, 130.13, 130.03, 130.00, 129.26, 129.16, 128.48, 127.71, 126.05, 125.62, 125.32, 124.57, 124.07, 123.79, 123.58, 122.74, 35.12, 34.72, 34.50, 34.39, 31.44, 31.35, 31.30, 31.11, 21.28, 20.15. HR-MS: calcd for $C_{68}H_{71}BF_2N_2$ $[M + Na]^+$: 987.5571; found 987.5566.

3 X-ray structure determination

The X-ray diffraction data were collected on a Bruker Smart Apex CCD diffractometer with graphite monochromated Mo Kα radiation (λ = 0.71073 Å) using the ω−2θ scan mode. The structure was solved by direct methods and refined on F^2 by full-matrix least-squares methods using SHELX-2000.[S1-S2] All calculations and molecular graphics were carried out on a computer using the SHELX-2000 program package and Mecury 2.4

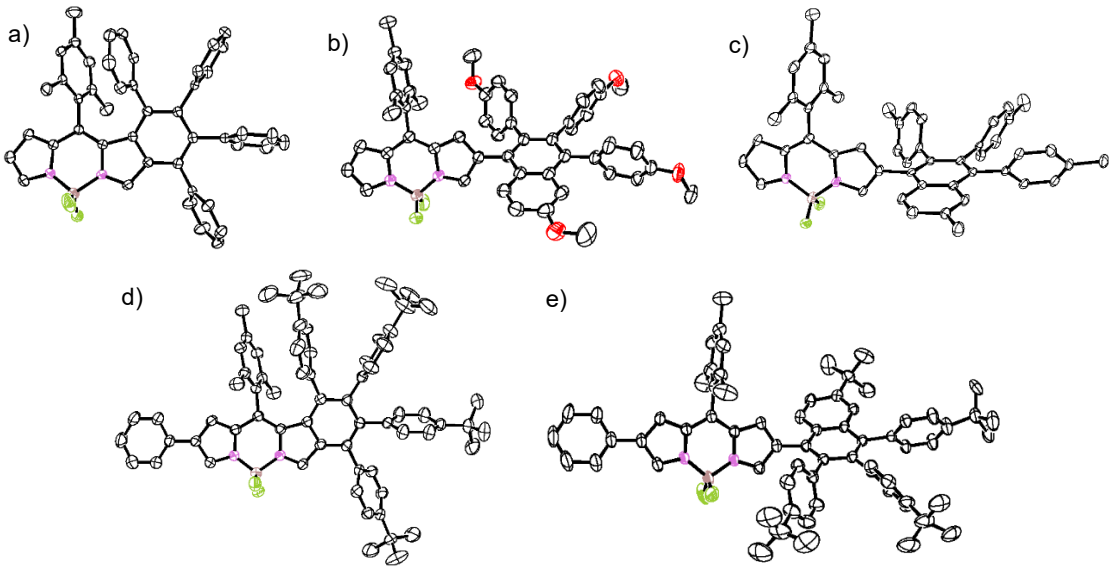


Figure S1. Crystal structures of BODIPYs **3a**, **4c**, **4d**, **3f** and **4f**. Thermal ellipsoids are scaled to 50% probability level. Atom's colour code: Carbon in black, nitrogen in pink, oxygen in red, boron in brown, fluorine in green. Hydrogen atoms are omitted for clarity.

Table S1. Crystal data and data collection parameters for BOPPYs **3a**, **3f**, **4c**, **4d** and **4f** obtained from crystallography.

	3a	**3f**	**4c**	**4d**	**4f**
CCDC. No.	1888818	2046853	2046854	1888819	2046855
formula	$C_{46}H_{35}BF_2N_2$	$C_{68}H_{71}BF_2N_2$	$C_{50}H_{43}BF_2N_2O_4$	$C_{50}H_{43}BF_2N_2$	$C_{68}H_{71}BF_2N_2$
fw	664.57	965.08	784.67	720.67	965.07
T (K)	153(2)	189.99	190(2)	173(2)	189.99
λ (Å)	0.71073	1.34138	1.34139	0.71073	1.34138
crystal system	Monoclinic	Triclinic	Triclinic	Monoclinic	Triclinic
space group	P2(1)/n	P -1	P -1	P2(1)/c	P -1
a (Å)	2.3636(17)	15.7803(6)	10.4208(4)	12.6316(7)	10.4968(4)
b (Å)	13.1822(17)	16.9989(6)	15.5643(6)	21.8885(14)	17.6320(7)
c (Å)	22.2800(3)	21.4911(8)	15.8333(7)	14.3585(8)	18.0969(7)
α (deg)	90	90.149(2)	115.241(2)	90	108.371(2)
β (deg)	100.247(3)	91.366(2)	96.172(2)	103.515(6)	99.158(2)
γ (deg)	90	90.205(2)	107.516(2)	90	97.864(2)
v (Å^3)	3573.2(8)	5763.2(4)	2130.73(15)	3860.0(4)	3075.0(2)
Z	4	2	2	4	2
D_{calcd} (mg/m^3)	1.235	1.112	1.223	1.240	1.042
μ mm^{-1}	0.078	0.337	0.426	0.078	0.316
F(000)	1396	2064	824	1520	1032
θ range (deg)	2.28-25.01	2.89-52.82	2.79-54.37	2.15-25.01	2.29-51.25
reflections collected / unique	20675/6282	62166/18381	28777/7886	15659/6543	32386/9936
R (int)	0.0494	0.0888	0.0457	0.0421	0.0448
goodness-of-fit on F^2	0.973	1.047	1.125	1.069	1.072
R_1, wR_2 [$I>2\sigma(I)$]	0.0490, 0.1236	0.0732, 0.1943	0.0461, 0.1447	0.0860, 0.1633	0.0687, 0.1913
R_1, wR_2 (all data)	0.0707, 0.1378	0.1041, 0.2243	0.0654, 0.1601	0.1176, 0.1849	0.0886, 0.2113
Largest diff. peak and hole, e. Å^{-3}	0.198/-0.214	0.364/-0.426	0.200/-0.184	0.357/-0.299	0.698/-0.504

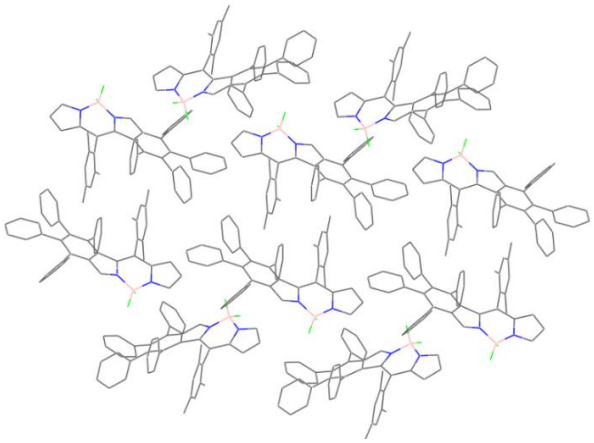


Figure S2. The crystal stacking diagram of **3a**, no π–π stacking interaction is found. Hydrogen atoms are omitted for clarity. Atom's colour code: Carbon in grey, nitrogen in blue, boron in pink, fluorine in green.

Table S2 Torsion angles [deg] for **3a**.

N2-C43-C42-C32	6.46	C31-C30-C25-C32	-7.60
C43-C42-C32-N1	7.54	C30-C25-C32-N1	9.11
C42-C32-N1-B1	-24.84	C26-C25-C30-C29	-7.60
C32-N1-B1-N2	24.52	C25-C30-C29-C28	1.31
N1-B1-N2-C43	-9.61	C30-C29-C28-C27	3.53
B1-N2-C43-C42	-4.15	C29-C28-C27-C26	-2.17
C32-N1-C31-C30	2.68	C28-C27-C26-C25	-4.03
N1-C31-C30-C25	3.30	C27-C26-C25-C30	8.63

4 Spectroscopic measurements

UV-Vis spectra were recorded on a Shimadzu 2550 spectrophotometer. Fluorescence spectra and absolute fluorescence quantum yields were measured on a Horiba FL spectrophotometer with a xenon arc lamp as light source. Fluorescence lifetimes were measured on a Horiba FL spectrophotometer with a 405nm laser as light source. Samples for absorption and emission measurements were contained in 1 cm × 1 cm quartz cuvettes. Photoluminescence measurements were conducted at a constant room temperature of (298 ± 2 K) throughout the study Dilute solution at a concentration of 10^{-5} M was used for the measurement of fluorescent quantum yields and fluorescence lifetime.

When the fluorescence decays were mono-exponential, the rate constants of radiative (k_r) and nonradiative (k_{nr}) deactivation were calculated from the measured fluorescence quantum yield (Φ_f) and fluorescence lifetime (τ) according to eqn (1) and (2):

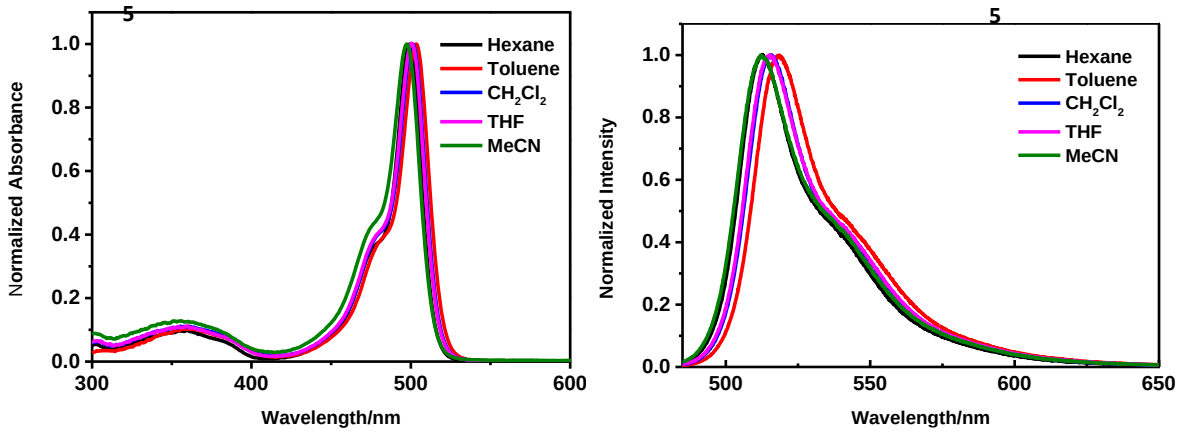
$$k_f = \Phi_f / \tau \qquad (1)$$

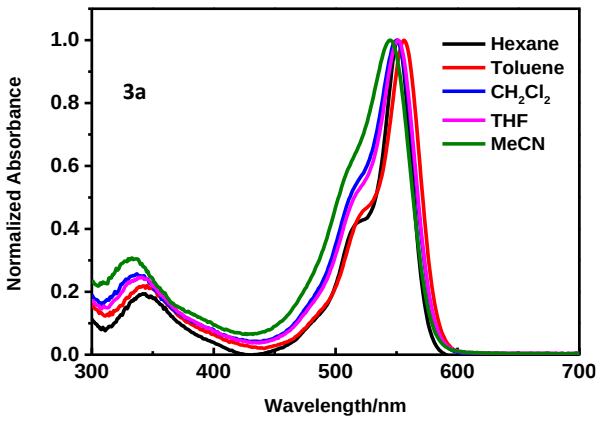
$$k_{nr} = (1-\Phi_f) / \tau \qquad (2)$$

Table S3 Photophysical properties of the unsymmetrical benzo[*a*]-fused BODIPYs **3a-3f**, naphthyl-BODIPYs **4c-4f** and the conrresponding unsubstituted BODIPY **5** in different solvents.

	Solvent	λ_{abs} [nm]	ε_{abs}	λ_{em} [nm]	$\Delta\nu_{em\text{-}abs}$ [cm^{-1}]	Φ_F	τ_f ns	κ_r 10^8 s^{-1}	κ_{nr} 10^8 s^{-1}
5	Hexane	499	69730	512	509	0.97	7.85	1.24	0.04
	Toluene	503	66860	518	576	0.93	6.18	1.50	0.11
	CH_2Cl_2	501	64030	516	580	0.93	7.04	1.32	0.10
	THF	500	65840	515	583	0.96	7.10	1.35	0.06
	CH_3CN	497	60270	512	589	0.95	7.34	1.29	0.07
3a	Hexane	551	80420	574	727	0.85	6.26	1.36	0.24
	Toluene	556	73060	583	833	0.85	5.39	1.58	0.28
	CH_2Cl_2	550	61060	581	970	0.89	5.98	1.49	0.18
	THF	551	79160	583	996	0.87	6.02	1.45	0.22
	CH_3CN	545	55300	580	1107	0.84	6.92	1.21	0.23
3b	Hexane	553	78090	577	752	0.83	6.08	1.37	0.28
	Toluene	559	71400	586	824	0.87	5.24	1.66	0.25
	CH_2Cl_2	552	59390	583	963	0.88	5.67	1.55	0.21
	THF	553	60680	581	871	0.85	5.69	1.49	0.26
	CH_3CN	546	52050	581	1103	0.86	6.14	1.40	0.23
3c	Hexane	556	59130	589	1008	0.82	6.44	1.27	0.28
	Toluene	563	56130	601	1123	0.80	5.37	1.49	0.37
	CH_2Cl_2	556	45270	604	1429	0.77	6.63	1.16	0.35
	THF	558	48380	599	1227	0.77	6.47	1.19	0.36
	CH_3CN	551	41820	607	1674	0.62	7.17	0.86	0.53
4c	Hexane	526	38830	622	2934	0.20	3.72	0.54	2.15
	Toluene	528	40210	647	3483	0.11	2.46	0.45	3.62
	CH_2Cl_2	526	39610	710	4927	0.01	0.76	0.13	13.03
	THF	525	40170	667	4055	0.02	2.49	0.08	3.94
	CH_3CN	521	41790	743	5735	<0.01	4.24	Nd	2.36
3d	Hexane	552	61840	578	815	0.93	6.40	1.45	0.11
	Toluene	558	57010	588	914	0.82	5.54	1.48	0.32
	CH_2Cl_2	552	47530	588	1109	0.87	6.24	1.39	0.21
	THF	554	50380	588	1044	0.79	6.17	1.28	0.34
	CH_3CN	546	44500	587	1279	0.95	6.85	1.39	0.07
4d	Hexane	523	39210	606	2619	0.24	3.79	0.63	2.01
	Toluene	527	39180	633	3178	0.20	2.56	0.78	3.13
	CH_2Cl_2	524	37390	664	4024	0.04	8.89	0.05	1.08
	THF	523	39160	649	3712	0.07	1.41	0.50	6.60

	CH_3CN	520	38200	703	5006	0.01	0.47	0.21	21.06
3e	Hexane	554	66530	579	779	0.86	6.37	1.35	0.22
	Toluene	560	61430	590	908	0.73	5.55	1.32	0.49
	CH_2Cl_2	553	49850	590	1134	0.71	6.18	1.15	0.47
	THF	554	54490	587	1015	0.71	6.08	1.17	0.48
	CH_3CN	549	44500	588	1208	0.79	6.81	1.16	0.31
4e	Hexane	523	42720	607	2646	0.27	3.87	0.70	1.89
	Toluene	526	43340	631	3164	0.22	2.93	0.75	2.66
	CH_2Cl_2	523	40760	682	4458	0.03	0.83	0.36	11.69
	THF	523	42710	652	3783	0.08	1.49	0.54	6.17
	CH_3CN	519	45000	705	5083	0.01	0.45	0.22	22.00
3f	Hexane	589	58160	620	849	0.73	5.39	1.35	0.50
	Toluene	594	53260	636	1112	0.52	4.33	1.20	1.11
	CH_2Cl_2	582	47180	636	1459	0.53	4.59	1.15	1.02
	THF	586	49780	635	1317	0.43	3.99	1.08	1.43
	CH_3CN	575	44080	638	1717	0.28	3.27	0.86	2.20
4f	Hexane	573	51670	630	1579	0.35	4.53	0.77	1.43
	Toluene	577	48000	641	1730	0.33	3.73	0.88	1.80
	CH_2Cl_2	571	46700	658	2316	0.06	1.20	0.50	7.83
	THF	573	47720	642	1876	0.27	2.30	1.17	3.17
	CH_3CN	565	48410	662	2593	0.01	0.614	0.16	16.12




3a
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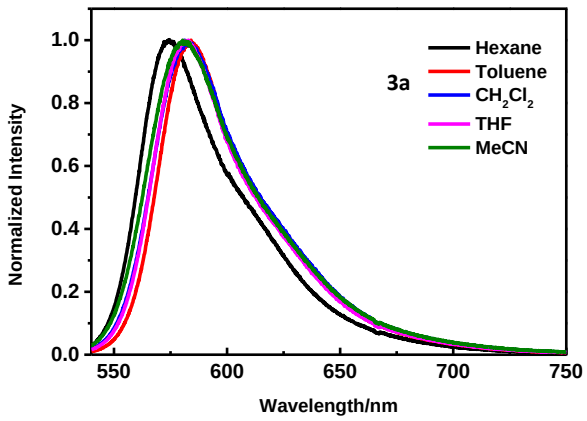
Toluene
CH_2Cl_2
THF
MeCN
Normalized Absorbance
Wavelength/nm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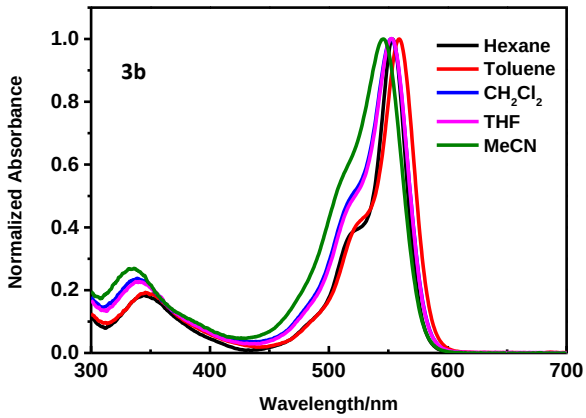
Toluene
CH_2Cl_2
THF
MeCN
Normalized Intensity
Wavelength/nm


3b
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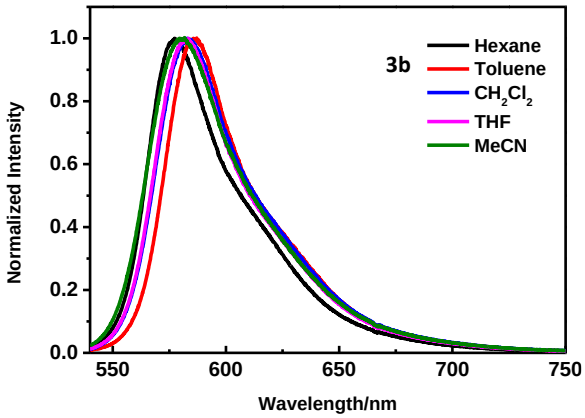
Toluene
CH_2Cl_2
THF
MeCN
Normalized Absorbance
Wavelength/nm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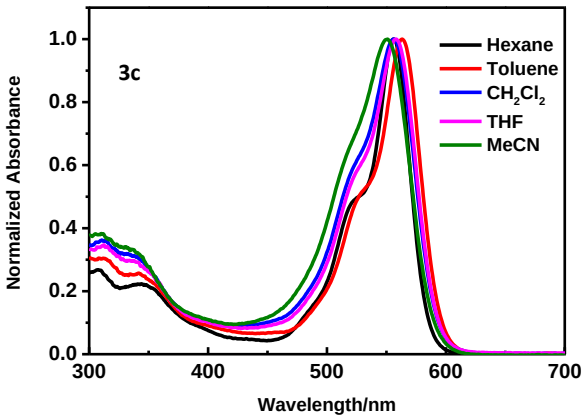
Toluene
CH_2Cl_2
THF
MeCN
Normalized Intensity
Wavelength/nm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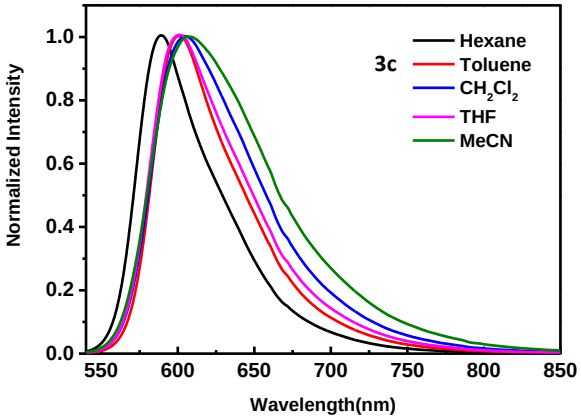
Toluene
CH_2Cl_2
THF
MeCN
Normalized Absorbance
Wavelength/nm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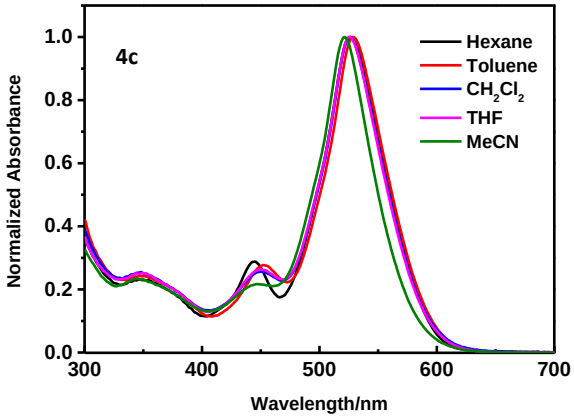
CH_2Cl_2
THF
MeCN
Normalized Intensity
Wavelength(nm)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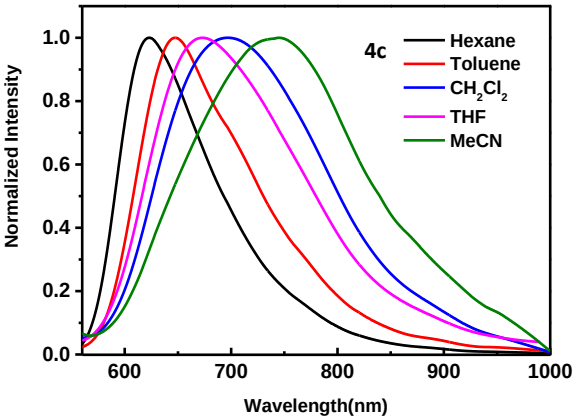
CH_2Cl_2
THF
MeCN
Normalized Absorbance
Wavelength/nm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THF
MeCN
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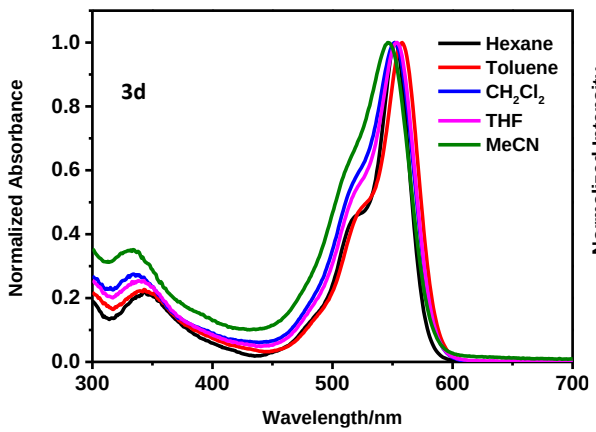
Wavelength(nm)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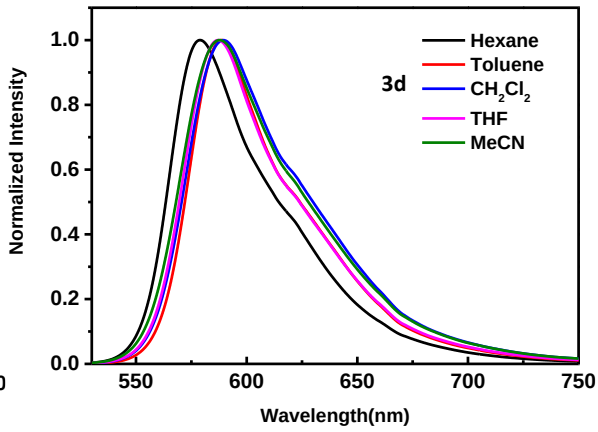
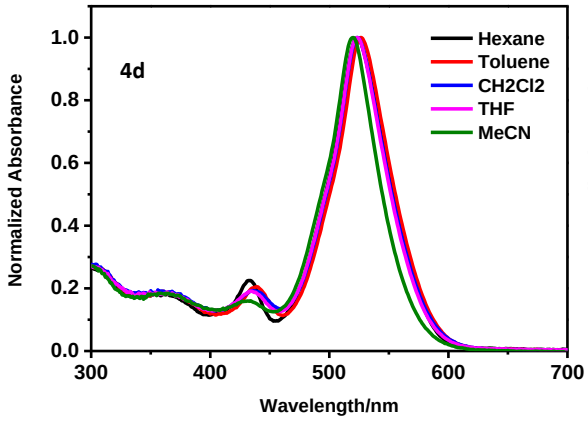
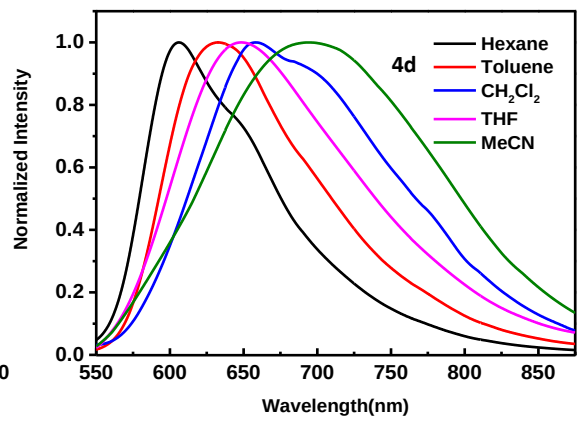
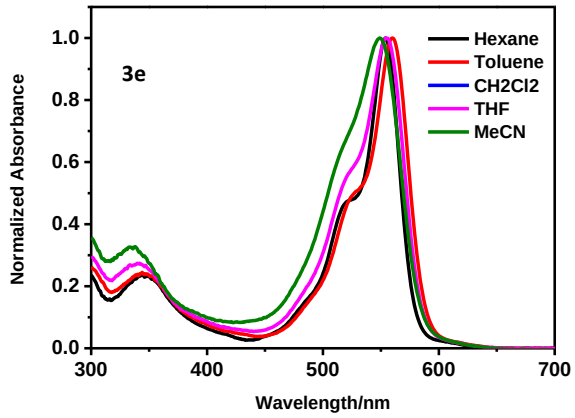
Hexane
Toluene
CH2Cl2
THF
MeCN
Normalized Absorbance
Wavelength/nm


3d
Hexane
Toluene
CH2Cl2
THF
MeCN
Normalized Intensity
Wavelength(nm)


4d
Hexane
Toluene
CH2Cl2
THF
MeCN
Normalized Absorbance
Wavelength/nm


4d
Hexane
Toluene
CH2Cl2
THF
MeCN
Normalized Intensity
Wavelength(nm)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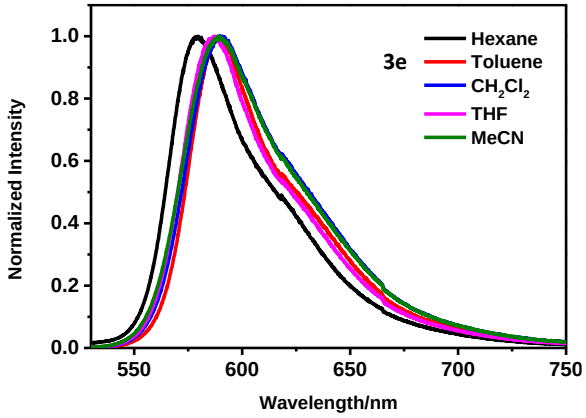
Hexane
Toluene
CH2Cl2
THF
MeCN
Normalized Absorbance
Wavelength/nm


3e
Hexane
Toluene
CH2Cl2
THF
MeCN
Normalized Intensity
Wavelength/nm

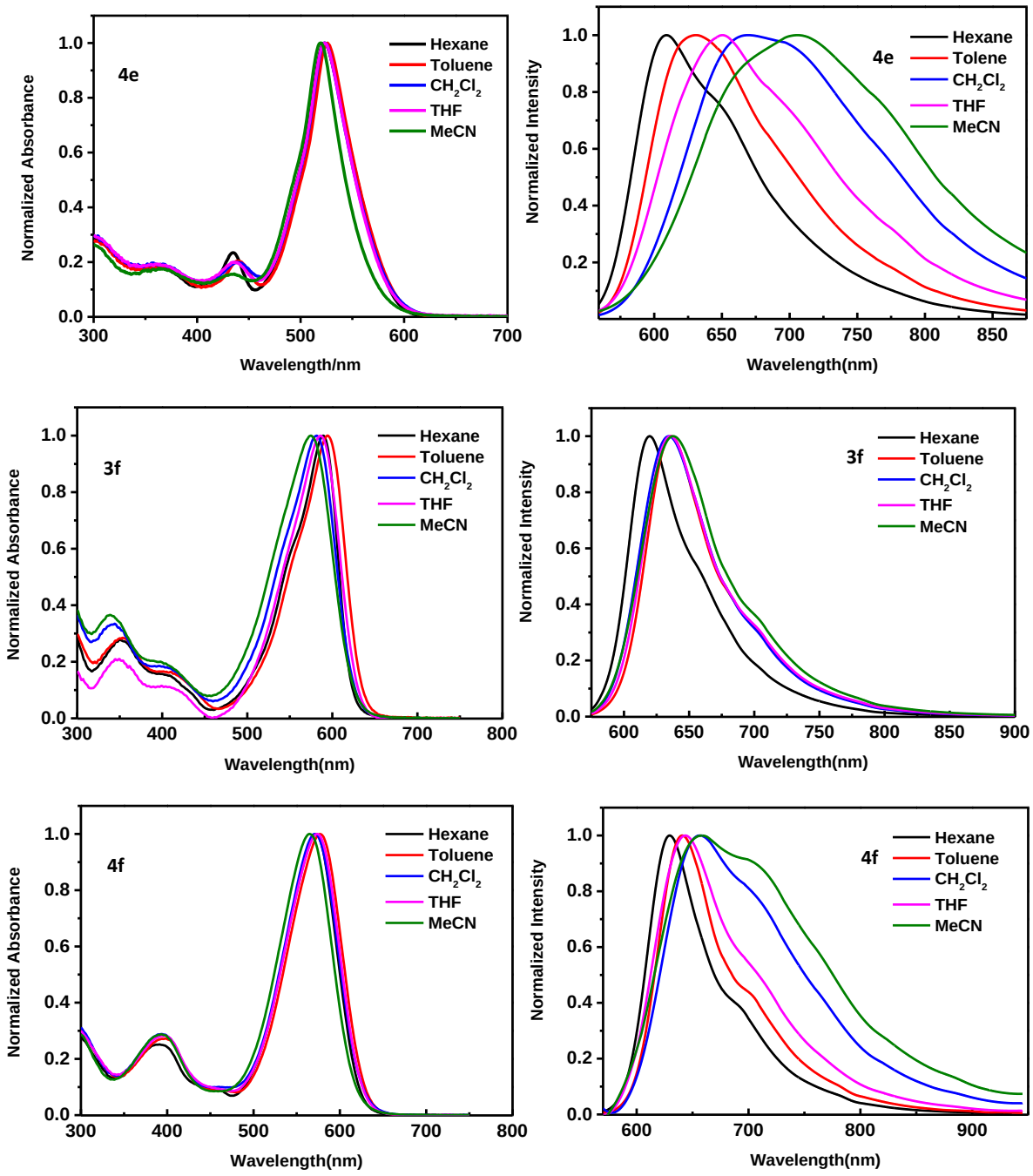


Figure S3. The absorption and emission spectra of **5**, **3a-3f** and **4c-4f** in different solvents.

6 Electrochemical properties

Table S4. Electrochemical data acquired and HOMO-LUMO gaps of selected compounds.

dyes	E_{ox} (V)	E_{red} (V)	E_{red}^{onset} (V)	E_{ox}^{onset} (V)	LUMO (eV)	HOMO (eV)[c]	E_g (eV)[d]
5	1.63	-0.75	-0.63	1.42	-3.77	-5.42	1.65
3a	1.20	-0.93	-0.82	1.10	-3.58	-5.10	1.52
3b	1.23	-0.89	-0.78	1.12	-3.62	-5.12	1.50
3c	1.13	-0.96	-0.85	1.02	-3.55	-5.02	1.47
3d	1.17	-0.96	-0.85	1.05	-3.55	-5.05	1.50
3e	1.18	-0.96	-0.85	1.05	-3.55	-5.05	1.50
4d	1.35, 1.42	-0.83	-0.73	1.23	-3.67	-5.23	1.56
4e	1.36, 1.44	-0.80	-0.68	1.26	-3.72	-5.26	1.54

E_{ox} = irreversible oxidation peak potentials; E_{red} = half-wave potential of the first reduction; E_{red}^{onset} = the onset reduction potentials; E_{ox}^{onset} = the onset oxidative potentials; $E_{LUMO} = -e(E_{red}^{onset} + 4.4)$; $E_{HOMO} = -e(E_{ox}^{onset} + 4.4)$; $E_g = E_{LUMO} - E_{HOMO}$.

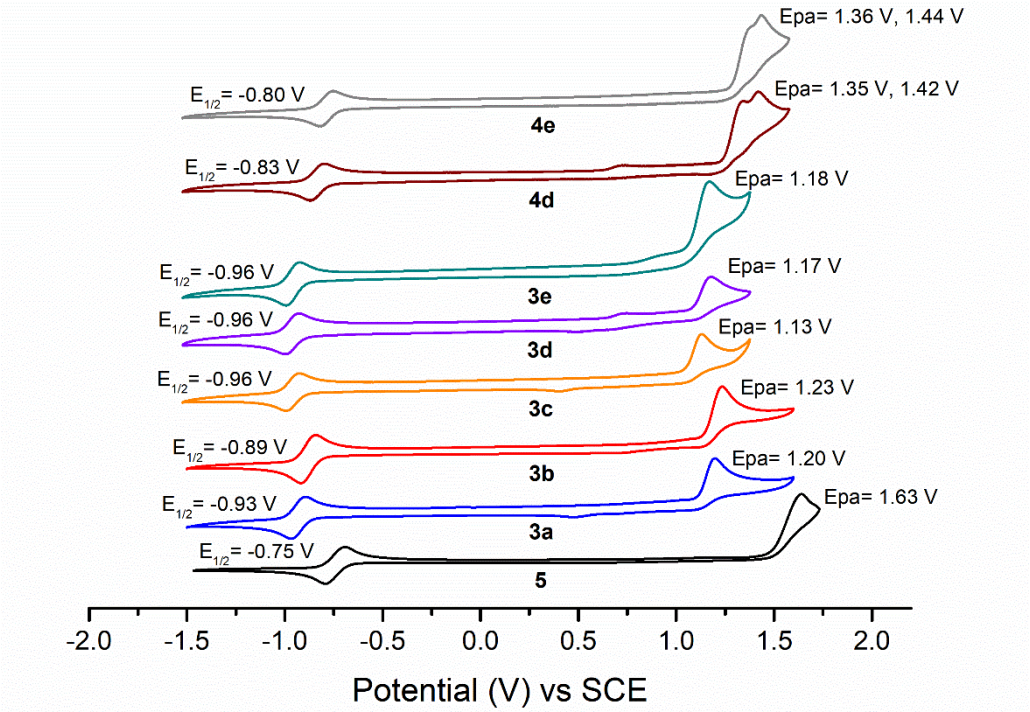


Figure S4. Cyclic voltammograms of selected BODIPYs(1 mM)measured in MeCN at a scan rate of 100 mVs^{-1}, containing0.1m $TBAPF_6$ as the supporting electrolyte at room temperature. Glassy carbon electrode as a working electrode.

6 Computational Details

The ground state structures of all reported products were optimized at DFT level using the CAM-B3LYP functional and the standard 6-31G(d) basis set.[S3] The absorption properties were predicted by time-dependent (TD-DFT) method by using the CAM-B3LYP functional with the same basis sets. For the mechanistic studies, the ground-state geometry optimizations of reported intermediates were conducted using B3LYP / GENECP, and the 6-31G(d) basis set for C, N, B, F, H and O, and SDD basis set for Pd, Br. All of the calculations were performed with the Gaussian09 program package.

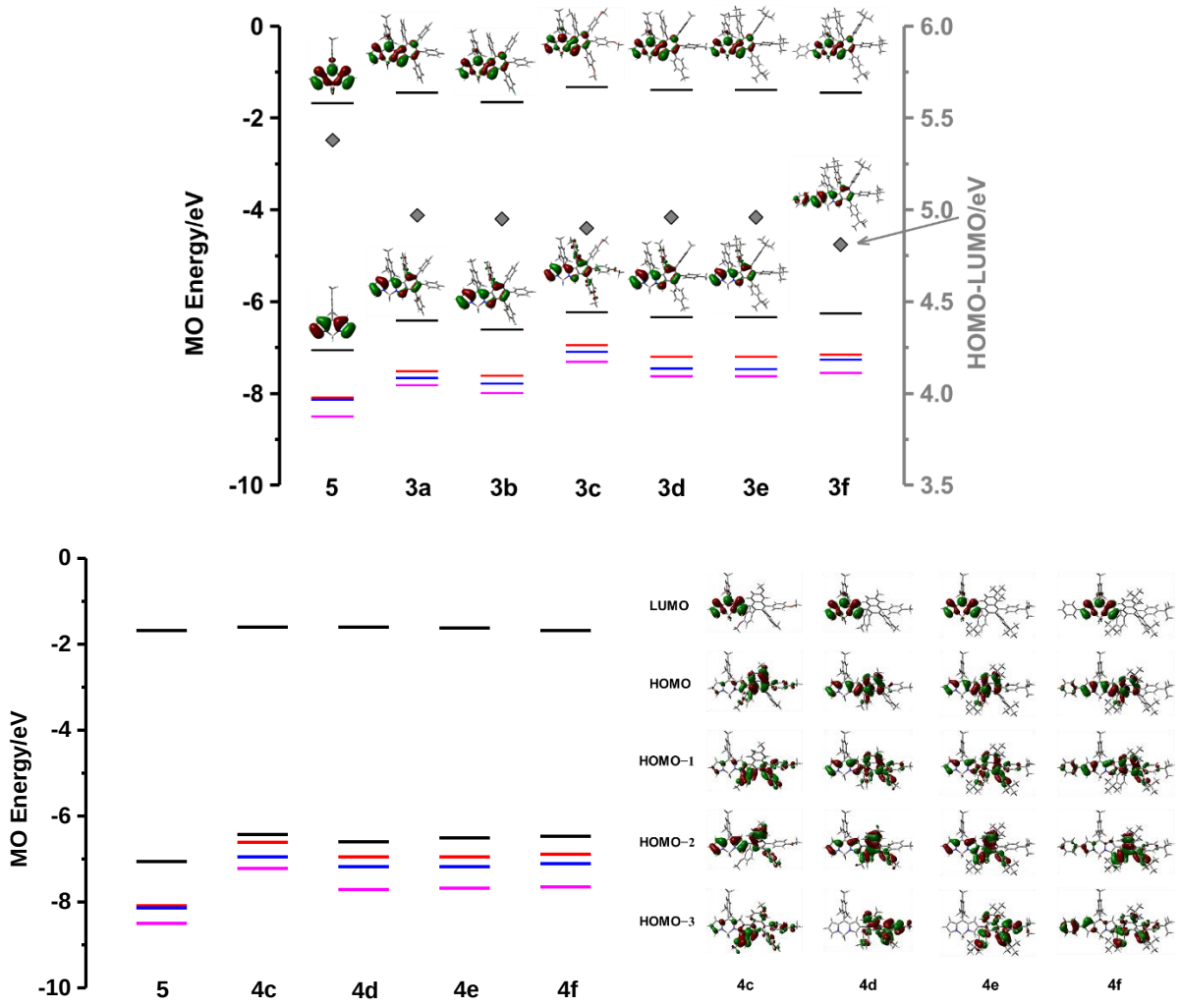


Figure S5. MO energies of selected BODIPYs. The HOMO-LUMO gaps are plotted against a secondary axis and are denoted with large diamonds. The red, blue and pink lines are used to denote the H-1, H-2, H-3 energy levels, respectively.

Table S5 Calculated electronic excitation energies, oscillator strengths, and eigenvectors for the TD-DFT spectra of classical BODIPY **5** and products BODIPYs **3a**-**3f**, **4c**-**4f**. Calculations were performed at the CAM-B3LYP/6-31G(d) level.

	State[a]	Energy [eV]	λ [nm]	f[b]	Orbitals (coefficient)[c]
5	S_1	3.17	392	0.4342	H→L (96%)
3a	S_1	2.82	440	0.6738	H→L (97%)
3b	S_1	2.81	442	0.6781	H→L (97%)
3c	S_1	2.79	445	0.6774	H→L (95%)
3d	S_1	2.81	442	0.6862	H→L (97%)
3e	S_1	2.81	443	0.6998	H→L (97%)
3f	S_1	2.68	464	0.8512	H→L (97%)
4c	S_1	2.90	428	0.5048	H→L (50%), H − 1→L (23%), H − 2→L (22%)
	S_2	3.38	368	0.1545	H→L (40%), H − 2→L (42%)
4d	S_1	2.90	423	0.5838	H→L (76%), H − 1→L (14%),
	S_2	3.55	350	0.1435	H→L (12%), H − 1→L (47%), H − 2→L (29%)
4e	S_1	2.86	435	0.5669	H→L (82%), H − 1→L (9%),
	S_2	3.50	355	0.1651	H→L (12%), H − 1→L (43%), H − 2→L (38%)
4f	S_1	2.72	456	0.7710	H→L (86%), H − 1→L (9%),
	S_2	3.40	366	0.1039	H→L (9%), H − 1→L (65%), H − 2→L (19%)
	S_3	3.78	328	0.1887	H − 1→L (4%), H − 2→L (13%), H − 3→L (40%), H − 4→L (14%), H − 5→L (12%)

[a] Excited state. [b] Oscillator strength. [c] MOs involved in the transitions.

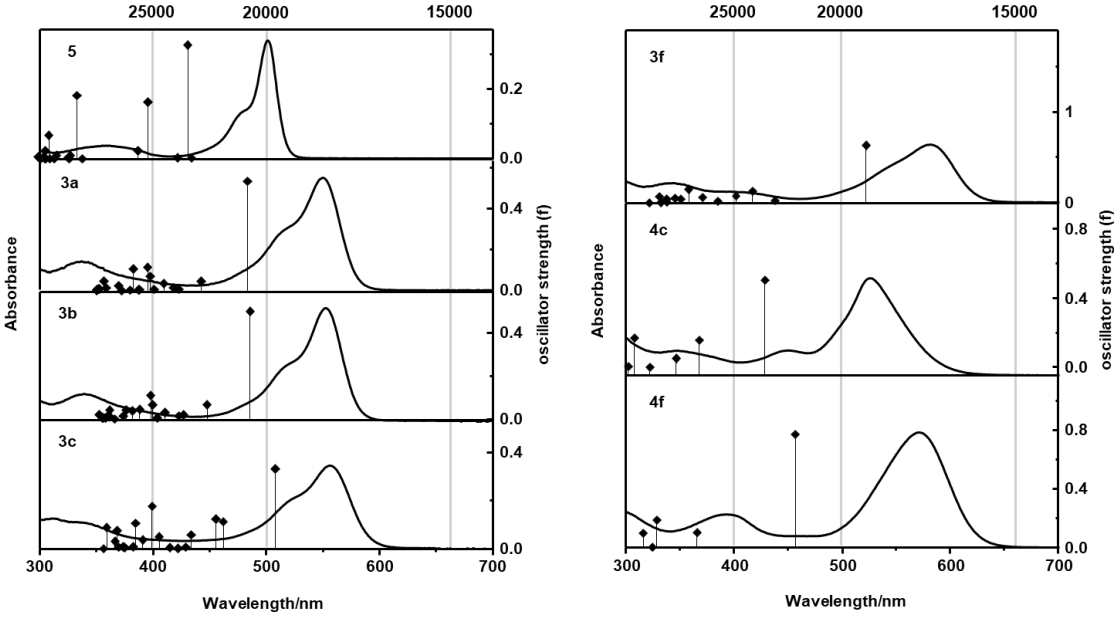
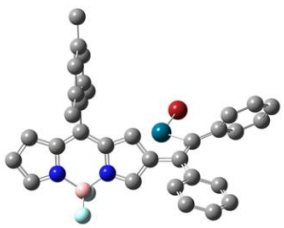
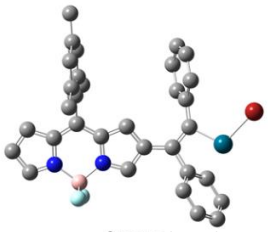


Figure S6. UV-vis absorption spectra and TD-DFT calculations for classical BODIPY **5** and selected BODIPYs. TD-DFT spectra calculated for CAM-B3LYP optimized geometries with the CAM-B3LYP functional and 6-31G(d) basis sets. The experimental absorption spectra in dichloromethane are plotted against a secondary axis.

Table S6 DFT Calculations of the regulatory effects of the substituents on the alkynes at b3lyp/genecp. Hydrogen atoms are omitted for clarity. For C, H, O, N, F, the 6-31(d) basis set was used, for Pd and Br the SDD was employed.



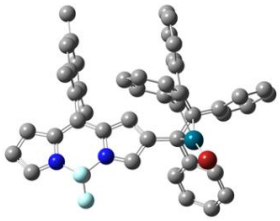
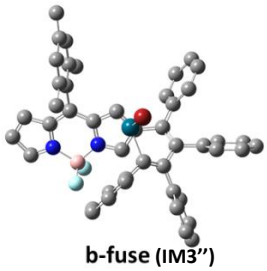
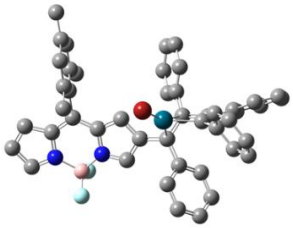
cis (IM2)



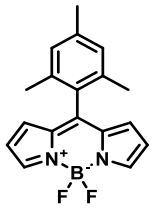
trans (IM2')

	Energy[a] (cis)	Energy[a] (trans)	ΔE (a.u.)	ΔE (kcal/mol)
R=F	-1908.589319	-1908.585467	0.003852	2.4
R=H	-1710.107656	-1710.104491	0.003165	2.0
R=OCH_3	-1939.086893	-1939.085995	0.000898	0.6
[a] Sum of electronic and zero-point Energies (Hartrees).				

Table S7 DFT Calculations of the origin of this totally a-Regioselectivity. Hydrogen atoms are omitted for clarity.

	 a-fuse (IM3)	 b-fuse (IM3'')	 naphthyl-link (IM3')
Energy[a]	-2249.407720	-2249.399394	-2249.412237
[a] Sum of electronic and zero-point Energies (Hartrees).			

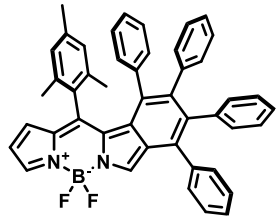
DFT optimized coordinates of BODIPYs **5**, **3a-3f** in the S0 geometry



BODIPY **5** in the S0 geometry

C	0.77426249	1.20936458	-0.02162151
N	2.16299612	1.24201970	-0.03563994
B	3.10902832	0.00340457	0.07781905
N	2.16593293	-1.23745804	-0.03548986
C	0.77711910	-1.20809581	-0.02142727
C	0.07818872	-0.00019697	-0.00757215
C	2.54762469	-2.51220808	-0.08949499
C	1.42553935	-3.36009271	-0.11109680

C	0.31120369	-2.54208277	-0.06669970
C	0.30519024	2.54221493	-0.06718958
C	1.41757826	3.36287560	-0.11170443
C	2.54166293	2.51766567	-0.08988892
F	3.73522798	0.00420689	1.30447842
F	4.01773768	0.00443872	-0.95489035
C	-1.41338592	-0.00171798	0.00405235
C	-2.09502527	-0.00456910	1.23006951
C	-3.48724433	-0.00942692	1.21857844
C	-4.21348731	-0.00872751	0.03131375
C	-3.51048473	-0.00988381	-1.16983352
C	-2.11864804	-0.00498353	-1.20851817
C	-5.71949524	0.01794269	0.04600273
C	-1.39764781	-0.00721239	-2.53272654
C	-1.34728482	-0.00645231	2.53924524
H	3.59806613	-2.76893940	-0.10954510
H	1.44975680	-4.43922871	-0.15766757
H	-0.72895777	-2.83642973	-0.07327882
H	-0.73566670	2.83403526	-0.07387276
H	1.43924802	4.44205716	-0.15848261
H	3.59149219	2.77688980	-0.10994759
H	-4.01813426	-0.01527564	2.16727464
H	-4.05977923	-0.01610083	-2.10799326
H	-6.11915265	-0.47839791	0.93468403
H	-6.09462598	1.04792662	0.05099991
H	-6.13649453	-0.47619049	-0.83591396
H	-2.10902031	-0.00806219	-3.36181596
H	-0.75454044	0.87196960	-2.64009697
H	-0.75493536	-0.88696317	-2.63781498
H	-2.04143272	-0.00714122	3.38279988
H	-0.70188383	0.87260887	2.63307177
H	-0.70227129	-0.88600445	2.63118955

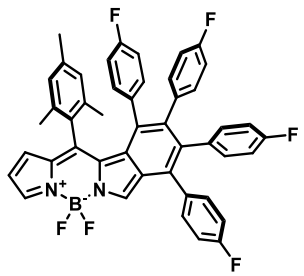


BODIPY **3a** in the S0 geometry

C	-3.72908196	2.02148800	0.21211500
N	-3.45496382	3.35097678	-0.04690289
B	-2.12638589	3.84642564	-0.62476605

N	-1.11294081	2.67732809	-0.31352892
C	-1.43830167	1.30693297	-0.23166598
C	-2.75017964	0.99520937	0.08665429
C	0.17707698	2.85254340	-0.21277616
C	0.83546711	1.59324280	-0.12229918
C	-0.16533872	0.59373171	-0.20558825
C	-5.05744413	1.93884413	0.66352487
C	-5.57593755	3.23218202	0.66383730
C	-4.55502337	4.07203406	0.22082300
F	-2.19308420	4.00094685	-1.99271591
F	-1.68406601	4.98981456	0.00037771
C	2.20108926	1.31274110	0.03472584
C	2.57286864	-0.02626608	0.11180300
C	1.59620395	-1.04462862	-0.07503930
C	0.23686880	-0.75819420	-0.27733905
C	-3.23372536	-0.36337375	0.47251687
C	-4.07296095	-1.07742891	-0.39611716
C	-4.63516446	-2.26994264	0.04767369
C	-4.40299728	-2.76244615	1.32828731
C	-3.58073816	-2.02680642	2.17474020
C	-2.98922004	-0.83179021	1.77219000
C	-5.00721101	-4.06857832	1.77170184
C	-2.13373169	-0.05951006	2.74496732
C	-4.39823148	-0.56436443	-1.77599178
C	-0.65798632	-1.83938239	-0.79089861
C	2.07463862	-2.46250196	-0.16350150
C	4.01479687	-0.38988923	0.27626672
C	3.16997475	2.44195089	0.10825957
C	-1.06949456	-1.76567460	-2.12413453
C	-1.77678120	-2.80886980	-2.71015196
C	-2.08693511	-3.94154847	-1.96779119
C	-1.69506063	-4.01721678	-0.63576853
C	-0.98568183	-2.97619711	-0.05248216
C	2.45254759	-3.00022755	-1.39324706
C	2.90574453	-4.31052657	-1.48413178
C	2.99126069	-5.10100285	-0.34395106
C	2.61996876	-4.57311381	0.88716756
C	2.16520029	-3.26301750	0.97487275
C	4.49359137	-0.90870166	1.47982903
C	5.83809820	-1.22431227	1.63255276
C	6.72455360	-1.02902618	0.57961766
C	6.25809873	-0.51387545	-0.62417186
C	4.91389683	-0.19523442	-0.77271729
C	3.95326870	2.65263878	1.24506029

C	4.82833402	3.72868046	1.31051438
C	4.93676420	4.61063643	0.24057963
C	4.16289432	4.41042491	-0.89612785
C	3.28382285	3.33547193	-0.95999165
H	0.60225984	3.84634427	-0.21340726
H	-5.55956142	1.03080801	0.96440126
H	-6.56818961	3.53999002	0.96089334
H	-4.54951591	5.14501985	0.08877709
H	-5.27767696	-2.82810340	-0.62899428
H	-3.40067578	-2.38524108	3.18545834
H	-6.03256724	-4.18021062	1.40650247
H	-5.02420100	-4.15289190	2.86173390
H	-4.43208762	-4.91811329	1.38446671
H	-2.20435842	-0.49248489	3.74591891
H	-1.07929812	-0.06763244	2.45054651
H	-2.44340037	0.98815582	2.80873199
H	-4.77958922	-1.37149779	-2.40624892
H	-5.15796525	0.22315630	-1.73672476
H	-3.51936408	-0.14009212	-2.26723128
H	-0.80994033	-0.88971209	-2.71155620
H	-2.07663771	-2.73784807	-3.75139139
H	-2.63167013	-4.76235131	-2.42441110
H	-1.93753341	-4.89614520	-0.04607960
H	-0.67863124	-3.04877404	0.98415930
H	2.38409064	-2.38664459	-2.28622604
H	3.19318624	-4.71457635	-2.44998286
H	3.34636350	-6.12449973	-0.41441811
H	2.68422081	-5.18260675	1.78353834
H	1.87304453	-2.85514314	1.93839247
H	3.80536027	-1.06156141	2.30549612
H	6.19355122	-1.62431694	2.57734031
H	7.77498552	-1.27677686	0.69726200
H	6.94307713	-0.35679102	-1.45176573
H	4.55459604	0.21494059	-1.71148954
H	3.87420845	1.96728166	2.08195761
H	5.42740739	3.87968381	2.20318320
H	5.62195168	5.45093408	0.29336733
H	4.24162196	5.09161985	-1.73771208
H	2.68573732	3.17833833	-1.85297336

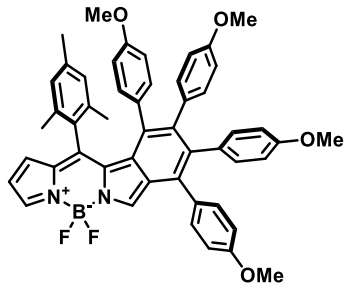


BODIPY **3b** in the S0 geometry

C	-3.82786196	2.50945351	0.25301590
N	-3.44775230	3.80298569	-0.05339360
B	-2.09354416	4.16530437	-0.66969574
N	-1.17631474	2.92445455	-0.33557152
C	-1.61270670	1.59097261	-0.20027977
C	-2.94292625	1.40186118	0.14823738
C	0.12635103	2.99508323	-0.27156322
C	0.67939911	1.68918197	-0.15219732
C	-0.40405711	0.77524968	-0.17470234
C	-5.15194008	2.55414125	0.72583208
C	-5.55928249	3.88484716	0.69131073
C	-4.47816829	4.62144993	0.20602451
F	-2.17354688	4.27806200	-2.04056070
F	-1.54391122	5.28599272	-0.09159776
C	2.02098515	1.29957631	-0.01819524
C	2.28208941	-0.06217008	0.10039993
C	1.21848089	-1.00055412	-0.02182192
C	-0.11630756	-0.60793819	-0.20362017
C	-3.53736522	0.10278223	0.58263887
C	-4.44324936	-0.56205068	-0.25381764
C	-5.10172659	-1.68971004	0.23341836
C	-4.90369033	-2.15565639	1.52739115
C	-4.00575244	-1.46936124	2.34200427
C	-3.31791777	-0.34588889	1.89624075
C	-5.64571142	-3.36028735	2.04458758
C	-2.38209992	0.37741041	2.83195938
C	-4.74177897	-0.06768520	-1.64667763
C	-1.11242607	-1.62759864	-0.65027249
C	1.57063311	-2.45688736	-0.06181776
C	3.69169030	-0.54252669	0.24003368
C	3.08435917	2.34232969	-0.01312673
C	-1.54578924	-1.57938503	-1.97759845
C	-2.36099360	-2.57267209	-2.50615315
C	-2.74127946	-3.61851445	-1.68579371
C	-2.33768553	-3.69690301	-0.36438108
C	-1.52269359	-2.69762924	0.14614000

C	1.87590671	-3.07583293	-1.27426172
C	2.20723691	-4.42331759	-1.32819510
C	2.23458301	-5.14781076	-0.14962286
C	1.94186541	-4.56828723	1.07215408
C	1.61065431	-3.21968570	1.10538224
C	4.15957217	-1.06821493	1.44546056
C	5.47313032	-1.49821675	1.58114348
C	6.31851944	-1.40006221	0.49000599
C	5.89224346	-0.88554877	-0.72163769
C	4.57636347	-0.45722923	-0.83656408
C	3.92098564	2.52233614	1.09157747
C	4.89280273	3.51251385	1.09906597
C	5.02430982	4.32550947	-0.01408811
C	4.21484593	4.17965481	-1.12637395
C	3.24413879	3.18574575	-1.11619177
F	-3.52935621	-4.58635465	-2.18414930
F	2.55412855	-6.45124615	-0.19240275
F	7.58980015	-1.81429114	0.61190572
F	5.96414066	5.28274469	-0.01304905
H	0.63067086	3.95002327	-0.31671533
H	-5.72345963	1.70167591	1.06310916
H	-6.51678406	4.28509625	0.99197562
H	-4.38561651	5.68553085	0.03860844
H	-5.79309538	-2.21440456	-0.42119180
H	-3.84252318	-1.81247814	3.36116448
H	-4.96790042	-4.06790294	2.53297375
H	-6.39942922	-3.07310984	2.78639955
H	-6.15975711	-3.88853875	1.23751070
H	-2.45882306	-0.03007773	3.84303297
H	-1.33919237	0.28634385	2.51174361
H	-2.61186964	1.44630404	2.88189543
H	-5.15709943	-0.87119387	-2.25994027
H	-3.84591066	0.30984713	-2.14512905
H	-5.46827480	0.75145597	-1.62683330
H	-1.22419552	-0.75958797	-2.61268507
H	-2.69516544	-2.54825826	-3.53725532
H	-2.66570118	-4.53042974	0.24606291
H	-1.20213308	-2.75193990	1.17952644
H	1.84737515	-2.49637209	-2.19146761
H	2.44268439	-4.91576787	-2.26479520
H	1.97586904	-5.17090421	1.97273218
H	1.37512949	-2.75319499	2.05736983
H	3.48705584	-1.13833524	2.29443699
H	5.84732801	-1.90568697	2.51346052

H	6.58672108	-0.82462291	-1.55181925
H	4.23056319	-0.04487107	-1.77903908
H	3.80936785	1.87921362	1.95740362
H	5.54513494	3.66351968	1.95156990
H	4.35052722	4.83530018	-1.97889371
H	2.60697952	3.05574921	-1.98571499

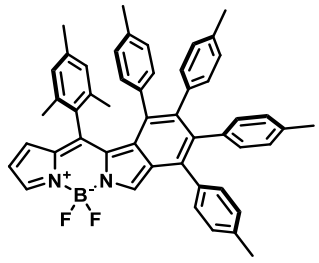


BODIPY **3c** in the S0 geometry

C	-3.76557393	-3.10933728	-0.31361027
N	-3.24794981	-4.33867837	0.04618114
B	-1.87565462	-4.52095917	0.69841943
N	-1.09781025	-3.19887244	0.33152019
C	-1.67949210	-1.92643802	0.14194265
C	-3.01193611	-1.90155787	-0.23226547
C	0.20421643	-3.12310347	0.27718394
C	0.61089985	-1.76819665	0.11384620
C	-0.56673212	-0.98061387	0.09697824
C	-5.06332900	-3.31963234	-0.80768398
C	-5.31860675	-4.68845220	-0.73228900
C	-4.17384197	-5.27963325	-0.20188722
F	-1.97074523	-4.59397641	2.07244102
F	-1.19011768	-5.59437684	0.17552367
C	1.90298364	-1.23957842	-0.02962480
C	2.01021706	0.13856353	-0.20738580
C	0.84746984	0.95601830	-0.13020565
C	-0.43802775	0.42505561	0.07022983
C	-3.74218713	-0.69334586	-0.71774253
C	-4.73604330	-0.11201566	0.08452046
C	-5.50803654	0.91624218	-0.44567603
C	-5.33555598	1.36937049	-1.75043219
C	-4.35626789	0.76434569	-2.52986231
C	-3.55244659	-0.26228857	-2.03877135
C	-6.17210176	2.50049534	-2.28709513
C	-2.52605985	-0.90147215	-2.93994723
C	-5.00084047	-0.60113299	1.48587827
C	-1.54603760	1.33850095	0.47946583

C	1.03273932	2.44205910	-0.16381162
C	3.35751952	0.76683998	-0.36396204
C	3.07210890	-2.15942752	0.01018207
C	-1.99637456	1.27546462	1.79535522
C	-2.92791622	2.18173934	2.29716844
C	-3.42719492	3.17768964	1.46425352
C	-2.98964990	3.25153607	0.14008967
C	-2.06450208	2.34613962	-0.34082024
C	1.28427719	3.15512633	1.00221824
C	1.46341097	4.53589908	0.98901251
C	1.39455182	5.22604497	-0.21807420
C	1.14631502	4.52412593	-1.39900887
C	0.96900149	3.15312358	-1.36581760
C	3.76469251	1.32850950	-1.57889463
C	5.02055817	1.88771838	-1.72611436
C	5.91049277	1.90515049	-0.65022184
C	5.52446443	1.35380210	0.56837851
C	4.25770919	0.79048682	0.69611281
C	3.96069282	-2.26540490	-1.06782622
C	5.02147186	-3.14886886	-1.03415278
C	5.23145965	-3.95648284	0.08719677
C	4.36277407	-3.86491834	1.17084967
C	3.29455715	-2.97216373	1.11921410
O	6.30144744	-4.79022573	0.02339647
C	6.54671337	-5.64307379	1.12031670
O	-4.33862152	4.11569666	1.84044274
C	-4.80903828	4.08589438	3.16885703
O	7.12069818	2.47647538	-0.89138965
C	8.05971543	2.51010265	0.15980147
O	1.55349095	6.57011883	-0.35066731
C	1.80938794	7.32607795	0.81155768
H	0.81246965	-4.01287654	0.35780401
H	-5.72004299	-2.54997139	-1.18668149
H	-6.21803874	-5.20444765	-1.03631921
H	-3.96413628	-6.31956594	0.00615777
H	-6.26957833	1.37537520	0.18028172
H	-4.21600139	1.09275808	-3.55693164
H	-6.11326143	2.56017192	-3.37724957
H	-7.22469040	2.38660532	-2.00998282
H	-5.83459759	3.46204690	-1.88293722
H	-2.64154512	-0.54549257	-3.96675650
H	-1.50596366	-0.66919689	-2.61757374
H	-2.62185088	-1.99161669	-2.94848903
H	-5.55139759	0.15020335	2.05766087

H	-5.59293171	-1.52213788	1.47760421
H	-4.07331049	-0.81967070	2.02053115
H	-1.59756228	0.51139502	2.45634882
H	-3.24497325	2.10004270	3.32958565
H	-3.39353106	4.03285199	-0.49456835
H	-1.73813727	2.42147294	-1.37115446
H	1.33777354	2.62593864	1.94870583
H	1.65421580	5.05491620	1.92017312
H	1.09779521	5.07870777	-2.32983035
H	0.77408963	2.61992492	-2.29212397
H	3.08500046	1.32072429	-2.42517834
H	5.33945237	2.32040772	-2.66809502
H	6.19421835	1.35177643	1.41944434
H	3.97028720	0.35376721	1.64761583
H	3.81300246	-1.64470673	-1.94474167
H	5.70742741	-3.23731351	-1.86945796
H	4.50202514	-4.47483668	2.05475754
H	2.62791380	-2.90299224	1.97403332
H	7.43107963	-6.22489772	0.85940435
H	6.74651890	-5.07403597	2.03642985
H	5.70537076	-6.32389620	1.29691050
H	-5.32297527	3.14319540	3.39460811
H	-5.51688788	4.91050426	3.25934307
H	-3.99449463	4.22905153	3.88946721
H	8.94787022	2.99834677	-0.24251042
H	8.32424706	1.50042586	0.49690342
H	7.68745331	3.08710907	1.01524181
H	1.90340593	8.36211001	0.48461393
H	0.98656544	7.24890539	1.53282442
H	2.74231941	7.01532592	1.29762557



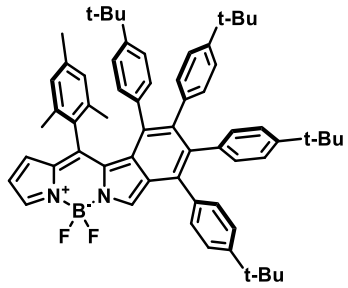
BODIPY **3d** in the S0 geometry

C	3.79601954	-2.56916351	0.19712513
N	3.40936735	-3.84214805	-0.17491272
B	2.06816779	-4.16091775	-0.84073434
N	1.15680732	-2.92583395	-0.47356345

C	1.60685721	-1.60123961	-0.27887220
C	2.92553843	-1.44304520	0.11063888
C	-0.14603844	-2.98279637	-0.41976827
C	-0.68685020	-1.67726976	-0.23853598
C	0.40290982	-0.77202293	-0.24853953
C	5.10251322	-2.65026354	0.70589246
C	5.49607158	-3.98555270	0.62603212
C	4.42300446	-4.68610666	0.07902589
F	1.49138010	-5.29943725	-0.32404323
F	2.18151374	-4.21870246	-2.21276392
C	-2.02509282	-1.28037765	-0.10650384
C	-2.28067814	0.08684570	-0.01902290
C	-1.21073495	1.01688497	-0.14060852
C	0.12817953	0.61068100	-0.28185883
C	3.52102492	-0.17112629	0.61753878
C	3.25489645	0.23072756	1.93578018
C	3.93912070	1.32763072	2.45233366
C	4.87472257	2.03183129	1.70152661
C	5.12735539	1.60522710	0.40190567
C	4.47447451	0.50894578	-0.15409889
C	5.57451914	3.23894940	2.26770433
C	4.82769145	0.05844703	-1.54893332
C	2.27656854	-0.51422101	2.80895493
C	1.16003143	1.62908480	-0.63767438
C	-1.54275267	2.47762436	-0.13526832
C	-3.68325852	0.56522222	0.18223167
C	-3.08787014	-2.32235242	-0.07692293
C	1.51201792	2.67721577	0.21287269
C	2.36564248	3.68076463	-0.21736263
C	2.89613725	3.67741153	-1.50818474
C	2.54539491	2.62881398	-2.35470488
C	1.69425447	1.61693255	-1.92630051
C	-1.95310110	3.10616168	1.03925812
C	-2.27157309	4.45813900	1.04919800
C	-2.19557170	5.22477288	-0.11204637
C	-1.79310123	4.59033210	-1.28735381
C	-1.46843669	3.24126404	-1.30038619
C	-4.35082258	0.29673140	1.37652157
C	-5.65834505	0.72232974	1.57463672
C	-6.34396107	1.42547655	0.58645505
C	-5.67715291	1.68458647	-0.61155898
C	-4.36944956	1.26637382	-0.81078258
C	-3.05656240	-3.33460509	0.88341348
C	-4.02397845	-4.33274932	0.89995557

C	-5.04883289	-4.35586038	-0.04256292
C	-5.07348039	-3.34560855	-1.00634402
C	-4.11479002	-2.34471512	-1.02433383
C	3.84244804	4.75988319	-1.95642846
C	-2.51481651	6.69701358	-0.09627641
C	-7.75238198	1.91162498	0.80894902
C	-6.11034603	-5.42406855	-0.01756530
H	-0.66363762	-3.92598864	-0.52396692
H	5.67344629	-1.82021366	1.09605904
H	6.43984486	-4.40980873	0.93737940
H	4.32165096	-5.74061338	-0.13650509
H	3.74007208	1.63327169	3.47675398
H	5.86170470	2.13614243	-0.19970932
H	5.05201587	4.16158192	1.98759622
H	5.61341399	3.20420935	3.36002916
H	6.59932343	3.32050226	1.89357770
H	5.26498639	0.88149637	-2.11970952
H	5.55287167	-0.76180816	-1.52718388
H	3.95150353	-0.30146604	-2.09286988
H	2.47821763	-1.58989264	2.81028563
H	2.33596419	-0.15929544	3.84087019
H	1.24543319	-0.37847212	2.46745787
H	1.09972096	2.71541005	1.21512965
H	2.62118839	4.48974928	0.46231963
H	2.93762042	2.60386091	-3.36811344
H	1.41874277	0.81880411	-2.60983998
H	-2.03295816	2.52809219	1.95489490
H	-2.59012795	4.92464789	1.97773557
H	-1.73109698	5.16282733	-2.20926471
H	-1.14583317	2.77491826	-2.22598599
H	-3.84178456	-0.25919734	2.15814863
H	-6.15580585	0.49932004	2.51485438
H	-6.19114849	2.22402323	-1.40300438
H	-3.87289200	1.48718323	-1.75024813
H	-2.27107869	-3.33620780	1.63364052
H	-3.97816126	-5.10793532	1.65999007
H	-5.85747191	-3.34575623	-1.75908716
H	-4.15722245	-1.57164600	-1.78393693
H	4.86090251	4.56486146	-1.59932788
H	3.88560107	4.82825609	-3.04696378
H	3.54557119	5.73860981	-1.56742339
H	-3.18381838	6.95182808	0.73041992
H	-1.60576943	7.29864863	0.02102158
H	-2.99348266	7.01241676	-1.02809765

H	-8.25569013	1.33433346	1.58945206
H	-7.76399425	2.96292637	1.11968098
H	-8.34986971	1.83777095	-0.10464609
H	-5.80447894	-6.27627395	0.59501686
H	-7.04908684	-5.03918112	0.39726557
H	-6.32897964	-5.79292647	-1.02433196



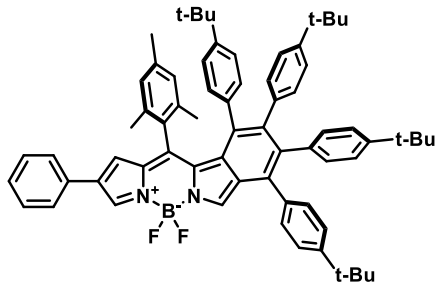
BODIPY **3e** in the S0 geometry

C	3.23519125	-4.31986787	0.42014820
N	2.48385516	-5.39238792	-0.02034405
B	1.16096217	-5.24901453	-0.77808529
N	0.67418332	-3.79028889	-0.42310741
C	1.51486700	-2.68808227	-0.15414418
C	2.78300891	-2.97144079	0.32119466
C	-0.57728260	-3.41986932	-0.44719518
C	-0.67605676	-2.01223078	-0.24898738
C	0.64694611	-1.51273320	-0.16304251
C	4.40577711	-4.82892349	1.00570908
C	4.35012138	-6.21835767	0.90258822
C	3.14900481	-6.52371025	0.26565787
F	0.21317110	-6.14605608	-0.33880991
F	1.34465499	-5.32119755	-2.14175980
C	-1.81809157	-1.20156315	-0.17819462
C	-1.61919480	0.17218175	-0.05244289
C	-0.29920154	0.70251862	-0.08030220
C	0.84109380	-0.11647968	-0.16204080
C	3.71568845	-1.96632510	0.91139714
C	3.49515147	-1.51711901	2.22285505
C	4.45403184	-0.70506801	2.82261494
C	5.62032658	-0.33300438	2.16229888
C	5.81910180	-0.80279305	0.86819652
C	4.89071666	-1.61901730	0.22890476
C	6.62833362	0.57330256	2.81806438
C	5.18055386	-2.13521386	-1.15783835
C	2.26828120	-1.91884202	3.00255412
C	2.16300669	0.51996848	-0.43885316

C	-0.13688396	2.19093190	-0.03936822
C	-2.79725921	1.08152029	0.09237814
C	-3.16133566	-1.83816509	-0.24957554
C	2.79067330	1.38823297	0.44827318
C	3.92421506	2.09853918	0.07177229
C	4.47201618	1.97877543	-1.20556781
C	3.84920445	1.08553480	-2.08283678
C	2.72317918	0.36724765	-1.70926229
C	-0.36710466	2.89774433	1.14115577
C	-0.21926867	4.27536069	1.18583936
C	0.15714724	5.01081158	0.05697865
C	0.37893300	4.29614242	-1.11982234
C	0.23656039	2.91356616	-1.16813696
C	-3.59027185	1.02852841	1.23985923
C	-4.68787493	1.86227128	1.38746433
C	-5.05028222	2.78160324	0.39749677
C	-4.25786828	2.82236067	-0.74944256
C	-3.15269721	1.99164182	-0.89915498
C	-3.52466842	-2.83178600	0.66379310
C	-4.76171574	-3.45357759	0.58624662
C	-5.68938088	-3.12023906	-0.40578569
C	-5.31703203	-2.12982920	-1.31536966
C	-4.08066930	-1.49955757	-1.24022843
C	5.68088509	2.79556712	-1.67590954
C	0.30800887	6.53308018	0.15007056
C	-6.26840535	3.68840262	0.60419810
C	-7.04401177	-3.83535337	-0.45666359
C	6.79381925	1.85450384	-2.16854430
C	5.24433017	3.71319118	-2.83261043
C	6.26056469	3.67312084	-0.56044646
C	-1.03477300	7.15609992	0.57145663
C	1.38135270	6.87776052	1.19783551
C	0.72624482	7.15830807	-1.18569278
C	-6.05015599	4.55753835	1.85555847
C	-7.52638731	2.82316734	0.79799775
C	-6.50906416	4.62033021	-0.58896168
C	-6.81827179	-5.34714147	-0.63715154
C	-7.80214665	-3.58679863	0.85960892
C	-7.91967973	-3.34097153	-1.61374586
H	-1.36470685	-4.14097729	-0.61572134
H	5.18584989	-4.23582656	1.46067921
H	5.08119702	-6.93104592	1.25649054
H	2.72687122	-7.48475302	0.00699048
H	4.28788660	-0.36440134	3.84185156

H	6.73054622	-0.53503050	0.33914784
H	6.45289321	1.62000300	2.54103631
H	6.57426329	0.51122102	3.90856412
H	7.64922067	0.32425153	2.51385164
H	5.91311823	-1.49811851	-1.65976011
H	5.58213639	-3.15338674	-1.12500962
H	4.27974840	-2.16462278	-1.77521952
H	2.10843540	-3.00094285	2.97002870
H	2.36635132	-1.62434496	4.05043570
H	1.36451054	-1.44555477	2.60561933
H	2.37883935	1.53155122	1.44121526
H	4.37151845	2.76821417	0.79669355
H	4.23725811	0.95424912	-3.08849813
H	2.24844992	-0.29872210	-2.42441259
H	-0.66968828	2.36098791	2.03533397
H	-0.40521462	4.78578187	2.12601721
H	0.67156262	4.81327832	-2.02603799
H	0.43235711	2.39010833	-2.09880754
H	-3.34359726	0.32145533	2.02631358
H	-5.27450379	1.78995744	2.29830720
H	-4.49269319	3.51231360	-1.55131288
H	-2.55548639	2.05985721	-1.80285151
H	-2.83321782	-3.11173710	1.45343731
H	-5.00503569	-4.21651155	1.31915771
H	-5.99487247	-1.83463490	-2.10721797
H	-3.82777171	-0.73343870	-1.96522230
H	6.45883968	1.22056809	-2.99434367
H	7.65283501	2.43454174	-2.52309794
H	7.13674860	1.20019783	-1.36087471
H	4.86389578	3.13821880	-3.68188392
H	4.45161664	4.39589550	-2.51008237
H	6.08995355	4.31364275	-3.18596680
H	5.53312092	4.40612691	-0.19794168
H	6.59773844	3.07457807	0.29221814
H	7.12566461	4.22665490	-0.93892726
H	-1.36968644	6.78190599	1.54311187
H	-0.94328211	8.24528651	0.64656671
H	-1.81651459	6.92945823	-0.16048703
H	1.11913231	6.49639380	2.18883181
H	2.34940771	6.44851168	0.92009869
H	1.50080871	7.96375892	1.27910095
H	0.82205945	8.24257299	-1.07096752
H	1.69254654	6.77559153	-1.52954547
H	-0.01399670	6.97319335	-1.97047398

H	-5.91654672	3.94853847	2.75421527
H	-5.16158589	5.18688840	1.74328054
H	-6.91324498	5.21178532	2.02099657
H	-7.43652317	2.16293638	1.66526758
H	-8.40556668	3.45850782	0.95207908
H	-7.70893859	2.19687204	-0.08100582
H	-5.65894128	5.28783560	-0.76185260
H	-6.69807854	4.06065150	-1.51049861
H	-7.38654243	5.24549080	-0.39624175
H	-6.23126531	-5.77222294	0.18188729
H	-7.77857832	-5.87339861	-0.66688129
H	-6.28723559	-5.55502447	-1.57136726
H	-7.24742681	-3.95995886	1.72523185
H	-7.98093295	-2.51769346	1.01222757
H	-8.77224386	-4.09533218	0.84106154
H	-8.14353477	-2.27293038	-1.52767756
H	-7.44676529	-3.51545684	-2.58535145
H	-8.87248305	-3.87943589	-1.60918310



BODIPY **3f** in the S0 geometry

C	4.39463495	-1.35226261	-0.05522209
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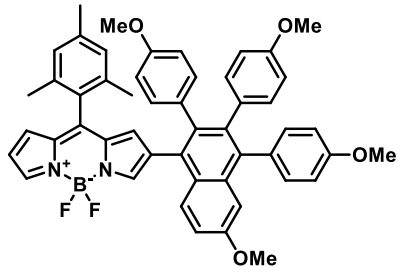
B	3.18997812	-3.29004613	-1.23989180
N	1.96395037	-2.41679792	-0.76824988
C	2.00961159	-1.03869077	-0.46065559
C	3.22822891	-0.52996945	-0.05071477
C	0.73675295	-2.85863251	-0.71938884
C	-0.15886189	-1.78900780	-0.42829719
C	0.61712458	-0.60571266	-0.36281510
C	5.67312725	-1.09106987	0.45403956
C	6.45494187	-2.23742605	0.25785723
C	5.61237294	-3.16921966	-0.36116165
F	2.99091358	-4.58792115	-0.82737935
F	3.28593958	-3.19286916	-2.61066396
C	-1.55103805	-1.81439942	-0.26430932
C	-2.19287180	-0.59291750	-0.06657057
C	-1.44514369	0.61630024	-0.11309622

C	-0.04884408	0.63362152	-0.28387365
C	3.42681212	0.81155192	0.57303820
C	3.06958273	0.99936309	1.91727992
C	3.40525612	2.20001719	2.53768544
C	4.08661620	3.20975436	1.86663010
C	4.43974912	2.99171818	0.53873861
C	4.12753294	1.80799972	-0.12276792
C	4.41241901	4.51262866	2.54769422
C	4.57209584	1.61004924	-1.54981245
C	2.36548312	-0.07406069	2.70885957
C	0.62339367	1.93667252	-0.56469538
C	-2.18969221	1.91059120	0.00399410
C	-3.66835040	-0.56272155	0.17342845
C	-2.26065667	-3.12128533	-0.31933427
C	0.67271321	2.97983633	0.35413425
C	1.14079918	4.23524278	-0.01456148
C	1.57028344	4.50327937	-1.31457451
C	1.54227838	3.44200545	-2.22467556
C	1.08409720	2.18483758	-1.85970416
C	-2.72372558	2.31657255	1.22716931
C	-3.41160103	3.51488317	1.34009311
C	-3.60541325	4.35740170	0.24036283
C	-3.07510040	3.93900829	-0.97963314
C	-2.37978762	2.74034938	-1.09657924
C	-4.20182313	-1.09994141	1.34601931
C	-5.56810774	-1.08496168	1.58015492
C	-6.46584212	-0.54262328	0.65469700
C	-5.92513754	-0.01425746	-0.51730216
C	-4.55468481	-0.02085554	-0.75310421
C	-1.90691181	-4.15678398	0.55021957
C	-2.53890407	-5.38941887	0.48536259
C	-3.54596318	-5.64919886	-0.44955354
C	-3.89031252	-4.61088272	-1.31568210
C	-3.26364449	-3.37197585	-1.25328506
C	2.02975574	5.89234401	-1.77145019
C	-4.36998147	5.67453872	0.41048739
C	-7.96896650	-0.54469767	0.95366135
C	-4.21463153	-7.02755250	-0.48944607
C	3.45623386	5.81306209	-2.34241098
C	1.07327972	6.40188444	-2.86511453
C	2.03163865	6.91072038	-0.62560379
C	-5.79077304	5.38077375	0.92417101
C	-3.63384230	6.56408891	1.42821098
C	-4.48916076	6.45199911	-0.90543632

C	-8.23548244	0.26542434	2.23500976
C	-8.45124801	-1.99205821	1.15726576
C	-8.78864851	0.07603269	-0.18350131
C	-3.15289245	-8.10105840	-0.78850192
C	-4.86572960	-7.32046698	0.87415742
C	-5.30177479	-7.11543159	-1.56690747
C	7.86005875	-2.44646518	0.63534618
C	8.43655620	-1.72490320	1.68569507
C	9.76492254	-1.91828936	2.04015121
C	10.54542887	-2.84510215	1.35768264
C	9.98411765	-3.57218847	0.31371124
C	8.65839397	-3.37115962	-0.04634518
H	0.51574486	-3.90065908	-0.90350200
H	5.98713431	-0.16093687	0.90517731
H	5.81508894	-4.19029890	-0.65290573
H	3.13613507	2.34254437	3.58156571
H	4.98518842	3.76243725	-0.00051865
H	3.65218424	5.27155475	2.32617604
H	4.45222578	4.39830916	3.63452404
H	5.37472081	4.91074503	2.21250564
H	4.77682590	2.57250961	-2.02528446
H	5.48389093	1.00598695	-1.60085150
H	3.81123744	1.09674517	-2.14254973
H	2.86581243	-1.04193898	2.60706542
H	2.34456601	0.18390520	3.77064117
H	1.33082086	-0.20735481	2.37713335
H	0.31970691	2.82020772	1.36703893
H	1.15126706	5.01753721	0.73513981
H	1.86822140	3.59722988	-3.24882367
H	1.04950064	1.38963729	-2.59920872
H	-2.60071902	1.68367228	2.10093729
H	-3.80742893	3.79520371	2.31159208
H	-3.19566472	4.55026375	-1.86621775
H	-1.96844424	2.45535482	-2.05991286
H	-3.53556543	-1.53785167	2.08334951
H	-5.93916190	-1.50952401	2.50806108
H	-6.57282525	0.41665300	-1.27152304
H	-4.17170880	0.40824102	-1.67357327
H	-1.13497352	-3.98938705	1.29596125
H	-2.23635134	-6.16403959	1.18312025
H	-4.66111435	-4.75717901	-2.06273564
H	-3.55961312	-2.58962252	-1.94381825
H	3.51925463	5.12787209	-3.19255235
H	3.78398147	6.80002200	-2.68669012

H	4.16248926	5.46823919	-1.58058820
H	1.06489966	5.73934034	-3.73538571
H	0.04846856	6.46780796	-2.48572605
H	1.37683206	7.39806162	-3.20556071
H	1.03148699	7.05174739	-0.20391957
H	2.70492401	6.60921725	0.18354550
H	2.37325990	7.88229140	-0.99619022
H	-5.77625426	4.86279762	1.88736758
H	-6.34931766	6.31403091	1.05585462
H	-6.33979491	4.75226544	0.21576606
H	-3.55654689	6.08250136	2.40716695
H	-2.61883011	6.79015512	1.08595933
H	-4.16716673	7.51150515	1.56330492
H	-5.04313128	7.38054685	-0.73570353
H	-3.50807244	6.72172790	-1.30923629
H	-5.02767724	5.88042693	-1.66798749
H	-7.70972109	-0.15444316	3.09735788
H	-7.90747716	1.30301656	2.11640158
H	-9.30627552	0.27046071	2.46687839
H	-7.93418003	-2.48071548	1.98790431
H	-9.52442407	-2.00806063	1.37688124
H	-8.27885788	-2.59152570	0.25776009
H	-8.51669692	1.12196638	-0.35728423
H	-8.66100392	-0.47175584	-1.12257277
H	-9.85244428	0.04954925	0.07262664
H	-2.36564631	-8.11697648	-0.02942677
H	-3.61357020	-9.09464817	-0.81255146
H	-2.67801652	-7.92276917	-1.75840234
H	-4.13152301	-7.31900105	1.68482339
H	-5.62857248	-6.57238879	1.11226985
H	-5.34595484	-8.30494098	0.86195464
H	-6.10393204	-6.39036912	-1.39627694
H	-4.89589234	-6.94871340	-2.56968281
H	-5.75054810	-8.11355826	-1.55495856
H	7.82930551	-1.01629108	2.24062922
H	10.19021711	-1.34737797	2.86028052
H	11.58313117	-2.99914940	1.63688643
H	10.58443167	-4.29468026	-0.23117525
H	8.23915033	-3.92555652	-0.88057458

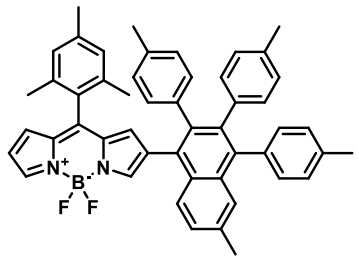


BODIPY **4c** in the S0 geometry

C	-5.33254935	-1.57176001	3.47608736
C	-4.98991828	-0.72447445	2.42556703
C	-5.03092716	-1.22761263	1.11672805
C	-5.41070640	-2.55501721	0.87067300
C	-5.74541937	-3.36465890	1.95272781
C	-5.70960873	-2.89420797	3.26223728
C	-6.04619282	-3.79954155	4.41817453
C	-4.59560805	0.70477006	2.70069453
C	-5.46290296	-3.10470583	-0.53232699
C	-4.66895778	-0.33390598	-0.02083448
C	-5.66245824	0.41355880	-0.66722822
N	-5.35407189	1.27009500	-1.71500420
B	-3.91974265	1.61978273	-2.20934713
N	-2.98313792	0.59672608	-1.48852133
C	-3.34702884	-0.24178761	-0.43910029
C	-7.05940051	0.44152065	-0.47614541
C	-7.58203718	1.31382066	-1.41845884
C	-6.49540286	1.80182205	-2.15950804
C	-1.67381460	0.48736556	-1.66009942
C	-1.11016340	-0.41720001	-0.72619554
C	-2.17307027	-0.88189058	0.02951028
F	-3.58257897	2.90511298	-1.81671089
F	-3.82957316	1.47623808	-3.57348781
C	0.34274714	-0.67337286	-0.56550201
C	0.88293599	-1.97792379	-0.77897356
C	2.28341878	-2.18813071	-0.63978936
C	3.13545702	-1.07904219	-0.32132162
C	2.58972161	0.17438315	-0.11645603
C	1.17663803	0.37540880	-0.22399693
C	0.07233362	-3.08045601	-1.13759667
C	0.59215524	-4.33604535	-1.31614830
C	1.97644187	-4.54808925	-1.13707705
C	2.79589796	-3.49390476	-0.80974924
C	0.56097057	1.71863052	0.00889152
C	3.46266450	1.34567996	0.19851780
C	4.60640044	-1.30458883	-0.20023780

C	-0.18597692	1.96250777	1.16566126
C	-0.92501205	3.12303941	1.31226627
C	-0.95267147	4.06713951	0.28479859
C	-0.16723958	3.86987341	-0.84873713
C	0.58755335	2.70772232	-0.97013807
C	4.37403945	1.83538983	-0.74364879
C	5.17792837	2.92541454	-0.46567566
C	5.09474612	3.55942482	0.77528090
C	4.19655021	3.08710162	1.72823398
C	3.39068026	1.99208338	1.42829526
C	5.25253070	-1.21051049	1.02818485
C	6.62405866	-1.41601894	1.15097120
C	7.37685351	-1.72301849	0.02069863
C	6.74504287	-1.82556313	-1.22037923
C	5.38110798	-1.62127687	-1.32300374
O	2.57692152	-5.76227017	-1.27353429
C	1.77912909	-6.87449073	-1.61108539
O	-1.76238996	5.14081032	0.47465693
C	-2.20161481	5.83205325	-0.68114599
O	5.92592792	4.62173911	0.95612421
C	5.86797227	5.30621030	2.18687023
O	8.71950579	-1.94041953	0.02196155
C	9.40671902	-1.83771492	1.24864148
H	-5.30510315	-1.18374230	4.49124981
H	-6.04332775	-4.39315400	1.76425802
H	-6.78963579	-4.54980624	4.13464313
H	-5.15759804	-4.33711454	4.76896096
H	-6.44090819	-3.23383265	5.26665292
H	-4.59363273	0.90667297	3.77439917
H	-3.59851039	0.93116308	2.30980827
H	-5.28788017	1.40762839	2.22599613
H	-4.48783470	-3.03664984	-1.02534751
H	-5.76645697	-4.15416033	-0.52720788
H	-6.17272878	-2.54974931	-1.15381251
H	-7.59619875	-0.13044828	0.26775267
H	-8.61942509	1.57525552	-1.56957679
H	-6.48787109	2.50501034	-2.98104368
H	-1.16782097	1.05953699	-2.42401723
H	-2.13279257	-1.58233695	0.85245740
H	-0.99041940	-2.92298290	-1.27827279
H	-0.06461360	-5.15183918	-1.59205539
H	3.85274011	-3.68881648	-0.68313076
H	-0.21658686	1.20718301	1.94581256
H	-1.52746510	3.30350589	2.19623305

H	-0.15635443	4.60045927	-1.64828103
H	1.17799296	2.55244931	-1.86872042
H	4.45378610	1.34791481	-1.71005919
H	5.88311775	3.30755011	-1.19579492
H	4.10903980	3.55992676	2.69866859
H	2.68833754	1.63874255	2.17667733
H	4.67546812	-0.96414556	1.91375293
H	7.08768725	-1.33196472	2.12613288
H	7.34787614	-2.06525768	-2.08960641
H	4.90108558	-1.70574478	-2.29364737
H	2.45740306	-7.72689421	-1.66212309
H	1.01305977	-7.07139489	-0.85101785
H	1.29248925	-6.74569063	-2.58569043
H	-2.97410685	6.52368924	-0.34206655
H	-1.39167003	6.40937198	-1.14348405
H	-2.62500081	5.13201208	-1.40879860
H	6.59797869	6.11362460	2.11984729
H	4.87335933	5.73290565	2.36538837
H	6.13161346	4.65122769	3.02659528
H	10.45514726	-2.03937795	1.02662052
H	9.31572271	-0.83297905	1.67914615
H	9.04478851	-2.57350826	1.97732420

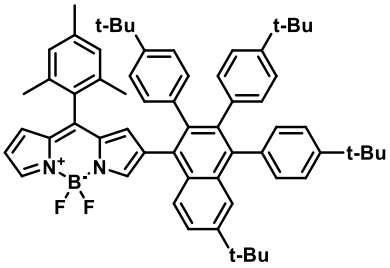


BODIPY **4d** in the S0 geometry

C	5.12685571	1.65258987	3.27986398
C	4.76339685	0.72492391	2.30698444
C	4.81594846	1.10979026	0.95918721
C	5.22714387	2.40139645	0.59827827
C	5.58094934	3.29466914	1.60572549
C	5.53459711	2.94193259	2.95143091
C	5.89177069	3.93733875	4.02406931
C	4.33233378	-0.66349258	2.70740451
C	5.29086087	2.82393052	-0.84747400
C	4.43510859	0.13395775	-0.10242414
C	5.40792065	-0.69479939	-0.67112345
N	5.08132703	-1.61630334	-1.65637760

B	3.68782945	-1.75767448	-2.34558375
N	2.71898629	-0.88916177	-1.47646286
C	3.10674274	0.02746704	-0.50527113
C	6.78404810	-0.82903339	-0.38504884
C	7.27232593	-1.83552062	-1.20140594
C	6.18762089	-2.29201848	-1.96858129
C	1.39965216	-0.81883117	-1.60067708
C	0.85973626	0.15281759	-0.72344009
C	1.94314792	0.68428304	-0.04182631
F	3.28351085	-3.07150029	-2.33958660
F	3.74339343	-1.24714227	-3.62422411
C	-0.57577857	0.49106684	-0.57322090
C	-1.02390490	1.81810164	-0.85931822
C	-2.39794496	2.14182961	-0.70853482
C	-3.32182077	1.12751750	-0.30640319
C	-2.87224320	-0.15399225	-0.04602573
C	-1.48319356	-0.47386520	-0.17291103
C	-0.14238969	2.83628835	-1.31218441
C	-0.58611084	4.10494002	-1.55677894
C	-1.94457930	4.45428293	-1.36265222
C	-2.81520944	3.47876465	-0.95175238
C	-1.01098828	-1.86080133	0.12585440
C	-3.83345903	-1.21764563	0.38024659
C	-4.76704919	1.47603720	-0.15459493
C	-2.40086279	5.86642813	-1.61310411
C	-0.19553841	-2.11606589	1.22877892
C	0.25909385	-3.40022288	1.49793713
C	-0.07691869	-4.47137795	0.67151706
C	-0.89899301	-4.21545038	-0.42542193
C	-1.36118996	-2.93439883	-0.69383353
C	-4.80169819	-1.70297365	-0.49834601
C	-5.69409002	-2.69023095	-0.10164042
C	-5.65258771	-3.22445639	1.18507263
C	-4.68819104	-2.73277593	2.06421145
C	-3.79084514	-1.75035971	1.66905898
C	-5.35991867	1.55326773	1.10577053
C	-6.70322675	1.87631029	1.24226093
C	-7.50043302	2.13587416	0.12788650
C	-6.90644299	2.05871634	-1.13104971
C	-5.56199606	1.73857351	-1.27143504
C	0.45399085	-5.85564583	0.93653002
C	-6.60175278	-4.31635541	1.60532515
C	-8.95136676	2.51139428	0.28201192
H	5.09064434	1.35593405	4.32511837

H	5.90252839	4.29550374	1.32842866
H	6.65889196	4.63709132	3.68061219
H	5.01769526	4.53029308	4.31740705
H	6.26436667	3.43903438	4.92330457
H	4.34829406	-0.77624996	3.79399095
H	3.31924494	-0.88611270	2.35765589
H	4.99079288	-1.42551605	2.27834675
H	4.31415200	2.73495865	-1.33383375
H	5.61826988	3.86252654	-0.93488761
H	5.98669737	2.20012131	-1.41725848
H	7.32574817	-0.24774990	0.34799421
H	8.28369266	-2.21269382	-1.24885942
H	6.16075202	-3.06743787	-2.72194102
H	0.87535665	-1.45447092	-2.30065393
H	1.92062589	1.44473990	0.72669075
H	0.90047266	2.59267724	-1.47279400
H	0.11201648	4.86156412	-1.90563161
H	-3.85925359	3.72922743	-0.80496121
H	-1.87670252	6.57423006	-0.96114989
H	-2.19810047	6.17169662	-2.64577482
H	-3.47338199	5.97658230	-1.43431761
H	0.08570283	-1.29602920	1.88299123
H	0.89043440	-3.57314377	2.36579419
H	-1.18178549	-5.03330766	-1.08289418
H	-2.00656482	-2.76440335	-1.55016623
H	-4.86037838	-1.29726339	-1.50353253
H	-6.43983915	-3.05008774	-0.80582727
H	-4.63755647	-3.12639627	3.07619227
H	-3.04473543	-1.39088916	2.37103077
H	-4.76232497	1.34738612	1.98815692
H	-7.14224447	1.92441495	2.23545435
H	-7.50600007	2.24920800	-2.01750603
H	-5.12119459	1.68465003	-2.26289313
H	0.67856053	-6.00171669	1.99698316
H	-0.26297267	-6.62413047	0.63311440
H	1.37977356	-6.03440090	0.37746919
H	-7.54591231	-4.25868245	1.05612564
H	-6.17417873	-5.30802659	1.41570085
H	-6.82817688	-4.25971041	2.67404766
H	-9.40277464	2.01490454	1.14588142
H	-9.06858132	3.59148865	0.42984766
H	-9.53065889	2.23953987	-0.60491698



BODIPY **4e** in the S0 geometry

C	-5.89182107	-2.39881518	3.37801302
C	-5.62387027	-1.39305018	2.45366251
C	-5.58661206	-1.72477834	1.09098027
C	-5.81806287	-3.04172277	0.66820769
C	-6.08266705	-4.01427340	1.62915473
C	-6.12034399	-3.71527113	2.98767562
C	-6.37728352	-4.79076566	4.01050781
C	-5.38438666	0.02081777	2.91904802
C	-5.78952815	-3.40957110	-0.79369393
C	-5.30475188	-0.66070014	0.08448944
C	-6.36095729	0.07568028	-0.46830926
N	-6.12879437	1.08016162	-1.39736619
B	-4.72998907	1.61844544	-1.81617240
N	-3.70940009	0.57482327	-1.25782565
C	-3.99760581	-0.40942454	-0.31613773
C	-7.75526414	-0.04334035	-0.29259491
C	-8.35178253	0.89133628	-1.12486737
C	-7.31182133	1.56180557	-1.78615939
C	-2.40034664	0.57298256	-1.46346198
C	-1.76000834	-0.40662376	-0.66101987
C	-2.77618671	-1.02255642	0.05210107
F	-4.50193031	2.84847448	-1.21503317
F	-4.63263386	1.70486129	-3.18331798
C	-0.29827503	-0.63279532	-0.55471437
C	0.23668701	-1.95005274	-0.71975595
C	1.63175165	-2.16576731	-0.56549502
C	2.49325364	-1.05633600	-0.28897651
C	1.96348957	0.21275213	-0.15870385
C	0.55349985	0.42649634	-0.28485206
C	-0.56657934	-3.06594217	-1.05963466
C	-0.03722999	-4.32285356	-1.18937733
C	1.34016884	-4.56757813	-0.98061766
C	2.13490479	-3.48581122	-0.67873148
C	-0.01421839	1.80356038	-0.16298871
C	2.85472509	1.37642071	0.13462848
C	3.95922806	-1.29666655	-0.12991899

C	1.95769139	-5.96847467	-1.08306983
C	-0.92217134	2.11984966	0.84431590
C	-1.59056509	3.33827947	0.85396747
C	-1.37583066	4.29369744	-0.13859423
C	-0.40782726	3.99771802	-1.10478704
C	0.25869126	2.78171304	-1.12134077
C	3.79715455	1.81525260	-0.79051653
C	4.62738153	2.89686476	-0.51468800
C	4.55291010	3.58087121	0.69770498
C	3.60314049	3.13302194	1.62253541
C	2.77032951	2.05965241	1.34925164
C	4.57567123	-1.20740815	1.11430246
C	5.94017866	-1.43834286	1.25914038
C	6.74384666	-1.76712793	0.16830746
C	6.11610269	-1.85805050	-1.07926953
C	4.75626666	-1.63183935	-1.22744422
C	-2.15663219	5.60998905	-0.20679087
C	5.45100034	4.77500777	1.03907802
C	8.25042747	-2.02225158	0.28738824
C	-3.30310188	5.64607603	0.81093738
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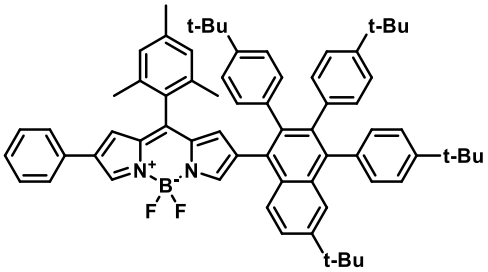

BODIPY **4f** in the S0 geometry

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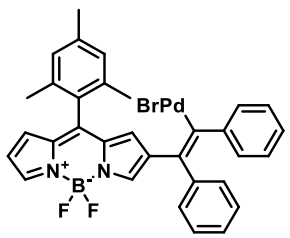
DFT optimized coordinates of the mechanistic study



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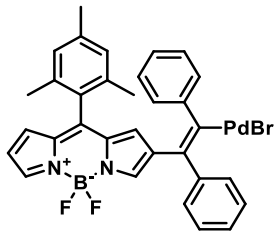

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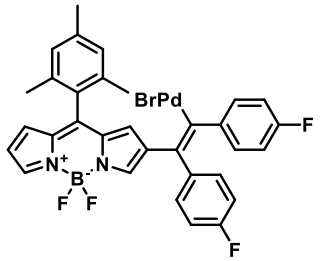

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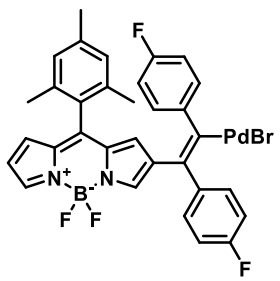

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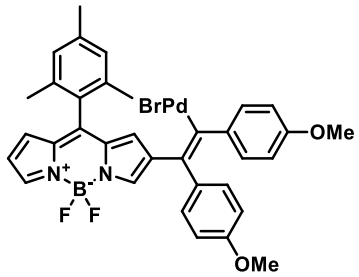

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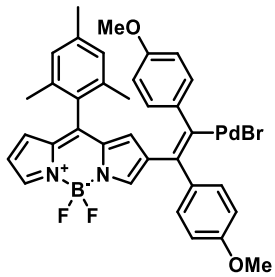

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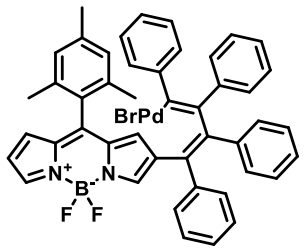

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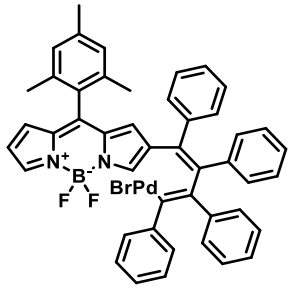

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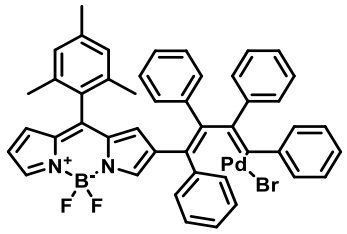

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Copies of ^{1}H and ^{13}C NMR spectra

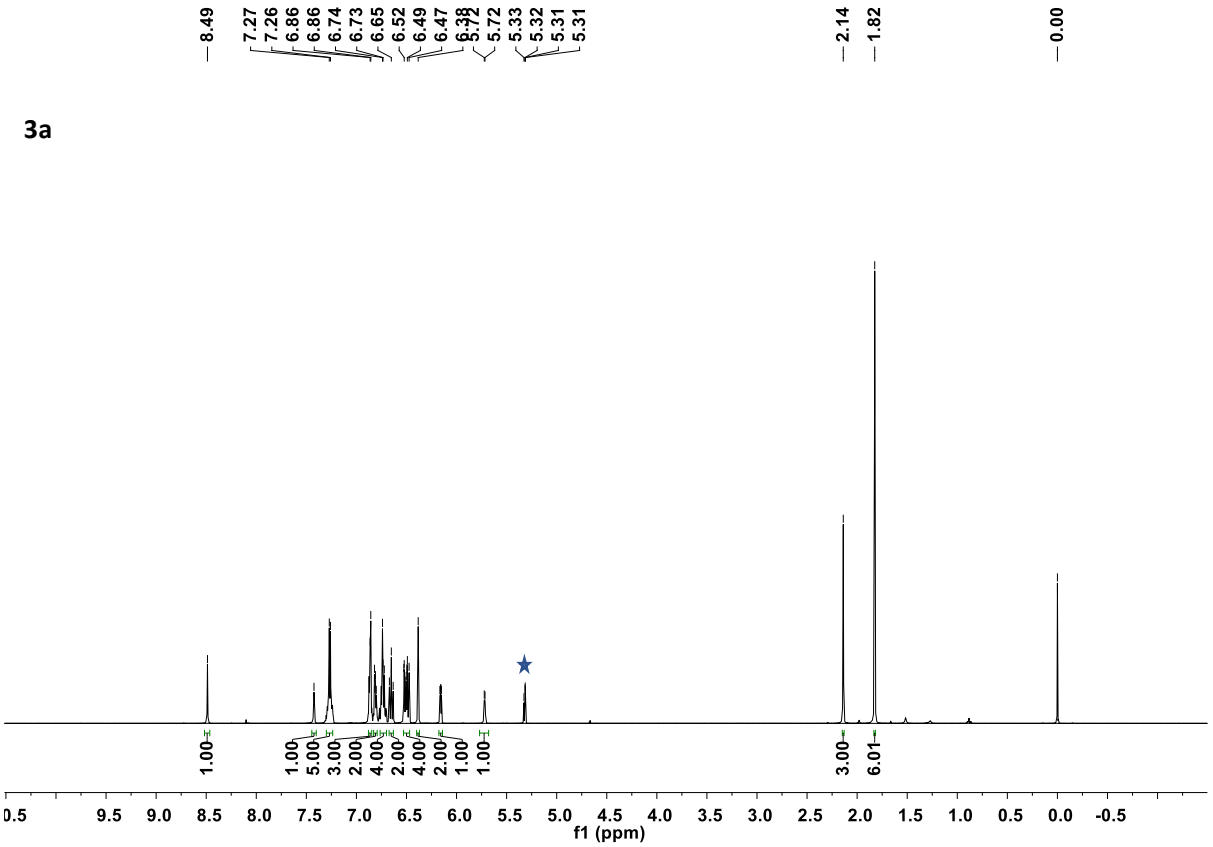


Fig S7 ^{1}H NMR spectra of the BODIPY **3a** (400 MHz, CD_2Cl_2).

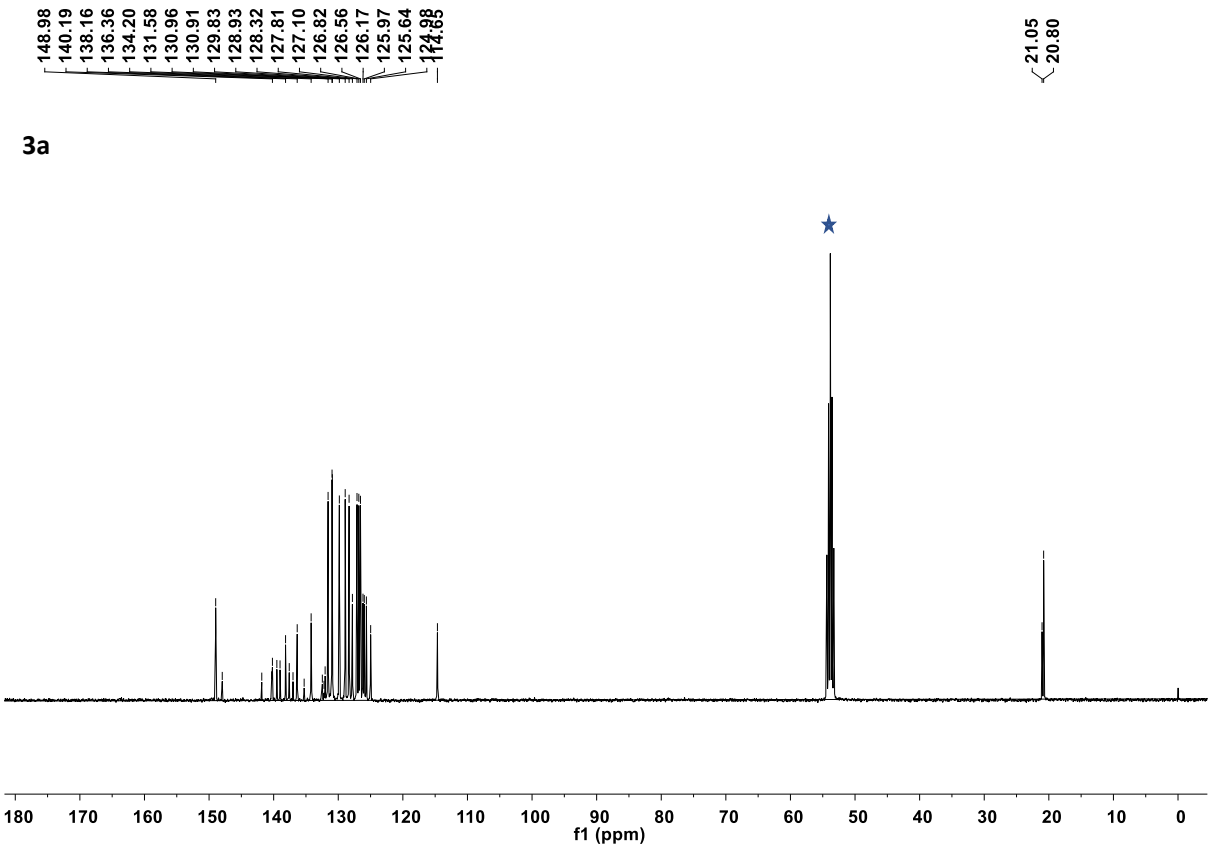


Fig S8 ^{13}C NMR spectra of the BODIPY **3a** (100 MHz, CD_2Cl_2).

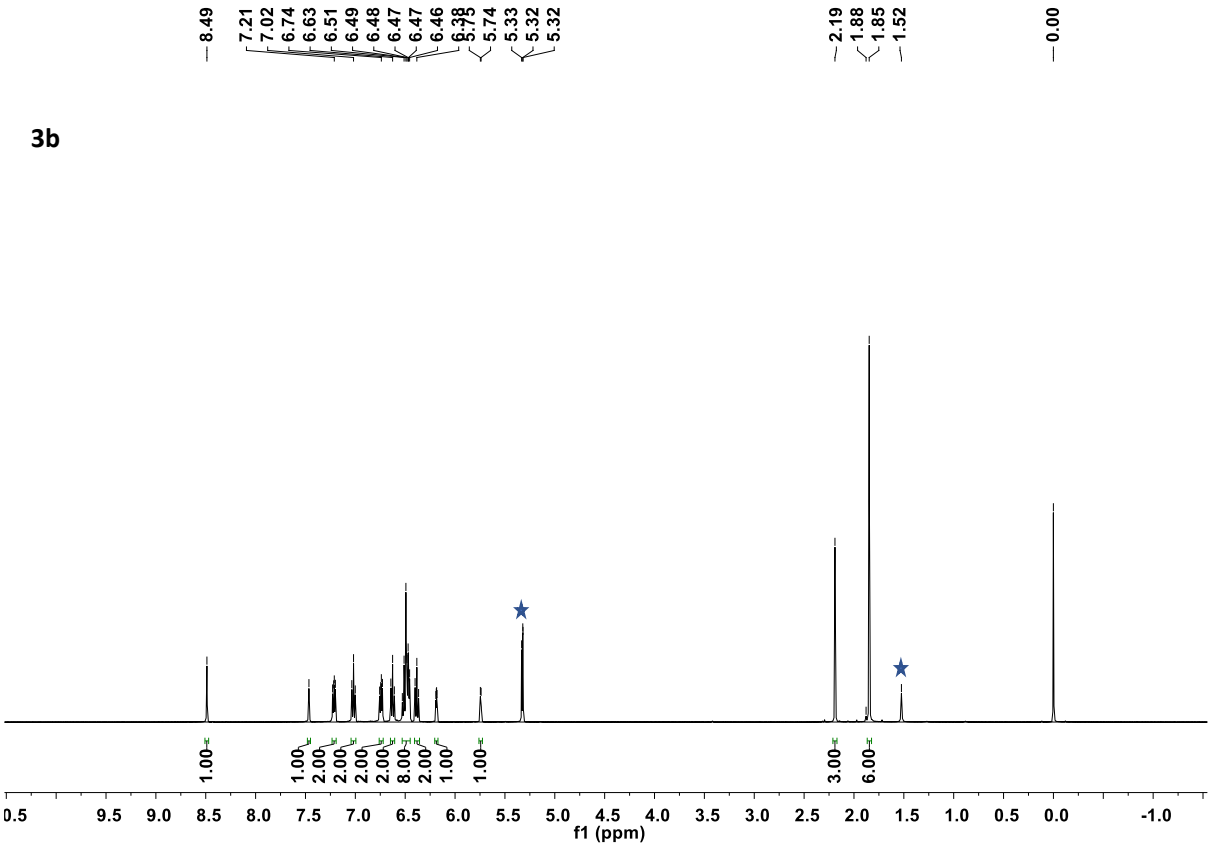


Fig S9 ^{1}H NMR spectra of the BODIPY **3b** (500 MHz, CD_2Cl_2).

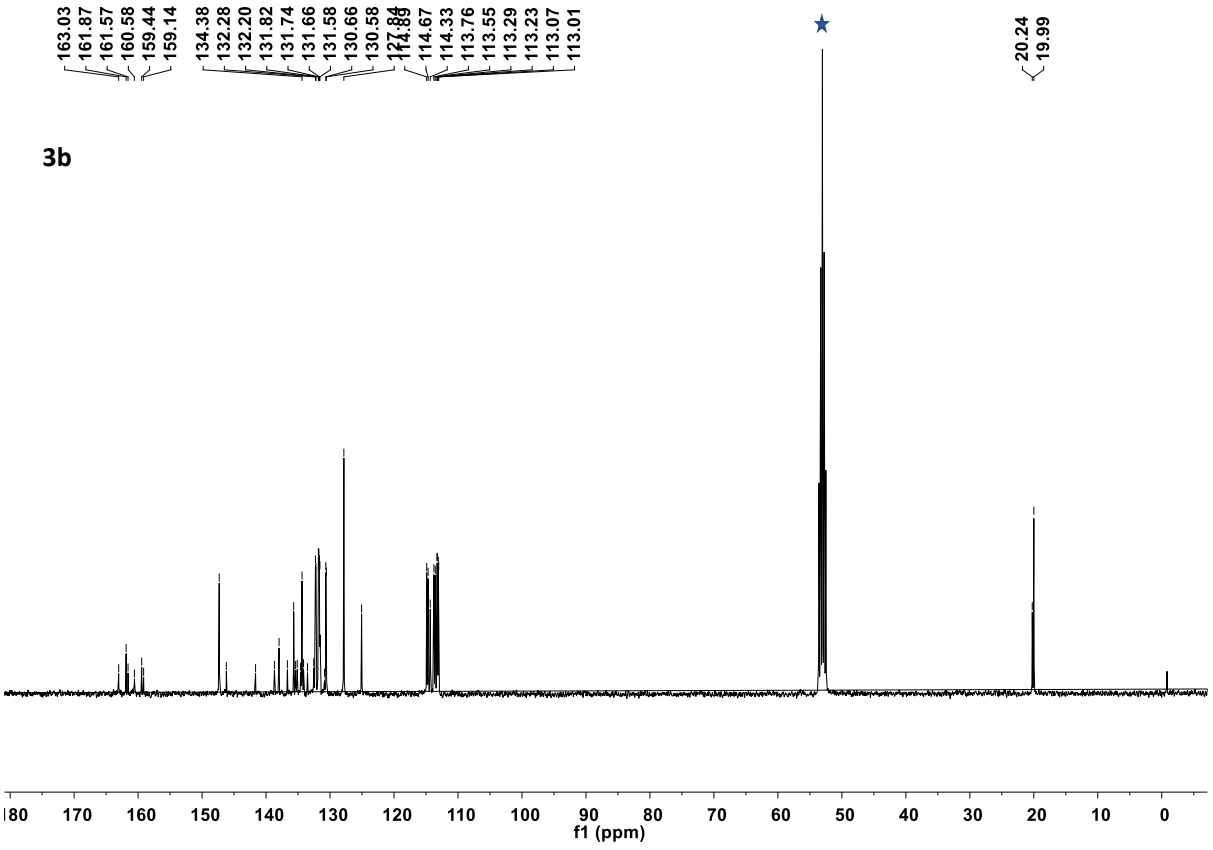


Fig S10 ^{13}C NMR spectra of the BODIPY **3b** (100 MHz, CD_2Cl_2).

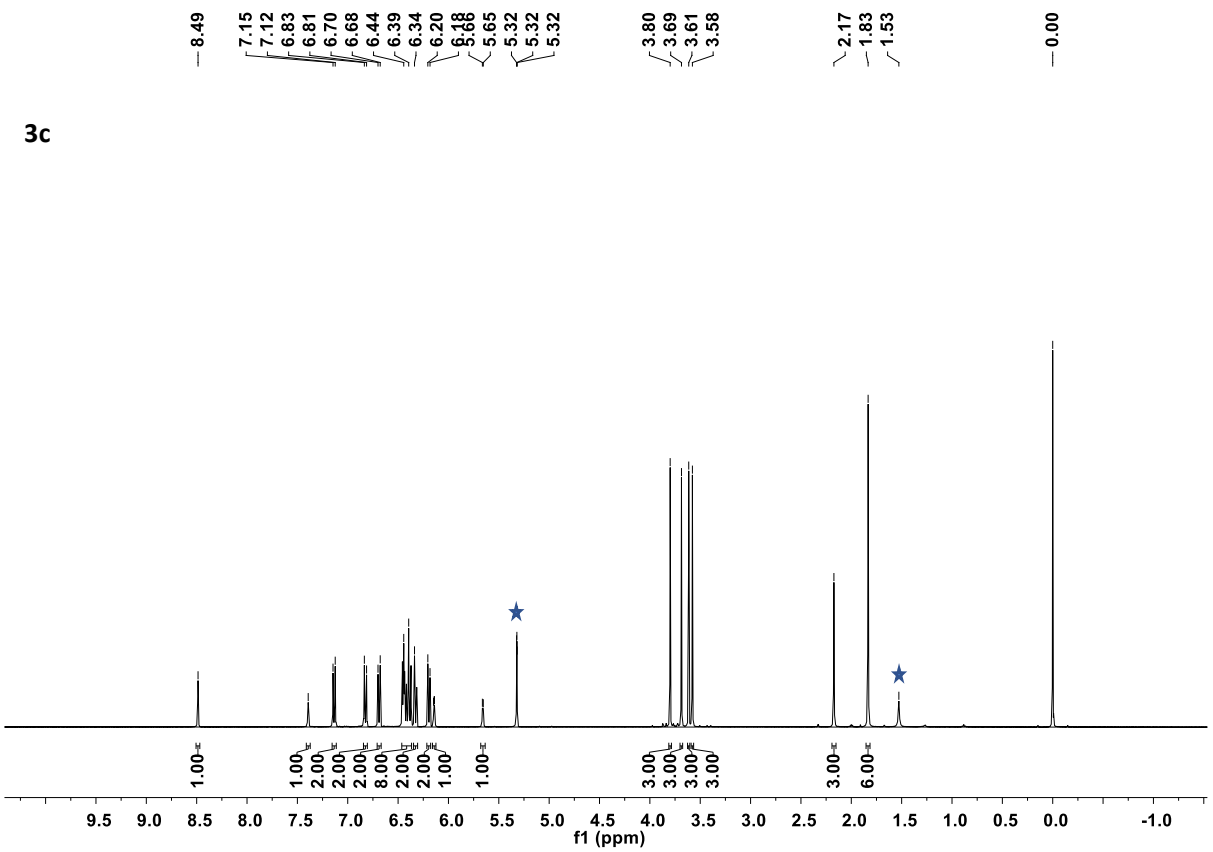


Fig S11 ^{1}H NMR spectra of the BODIPY **3c** (400 MHz, CD_2Cl_2).

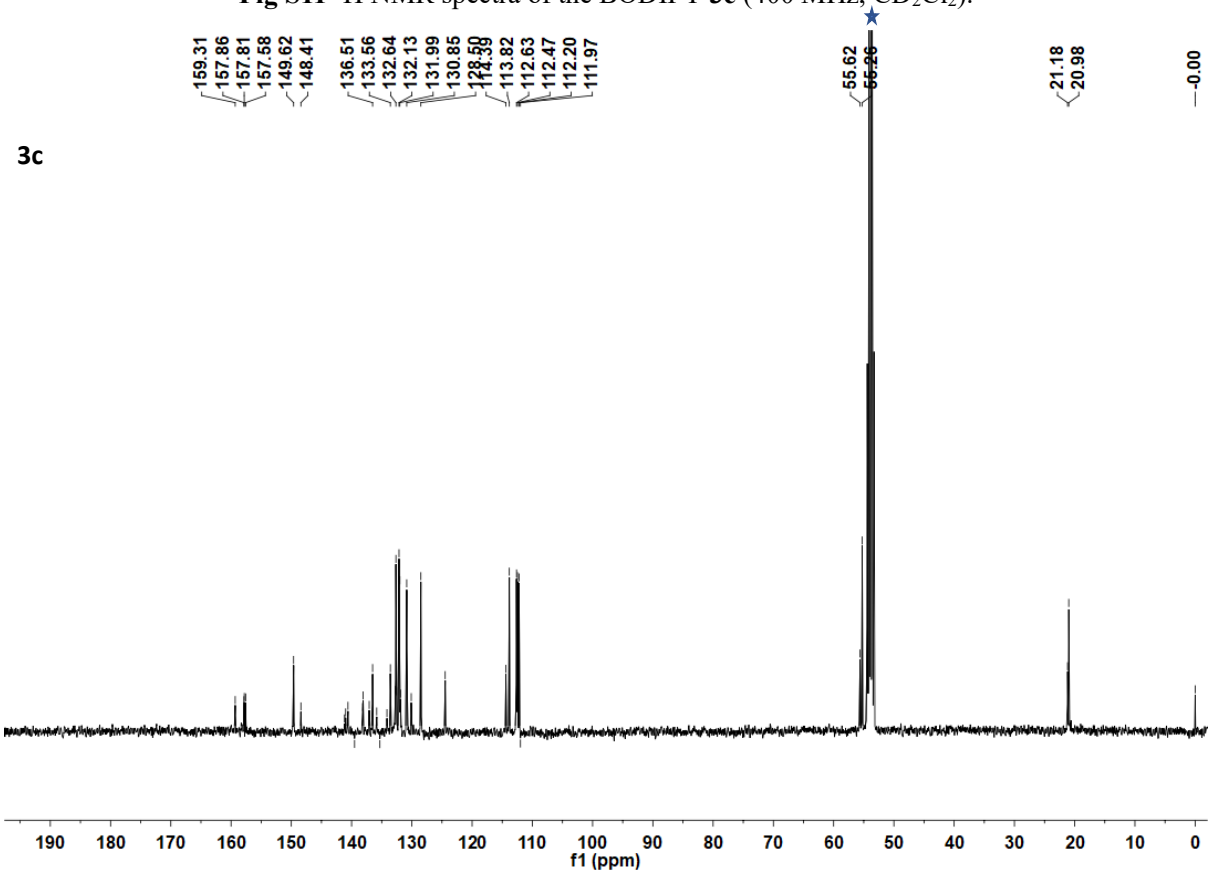


Fig S12 ^{13}C NMR spectra of the BODIPY **3c** (100 MHz, CD_2Cl_2).

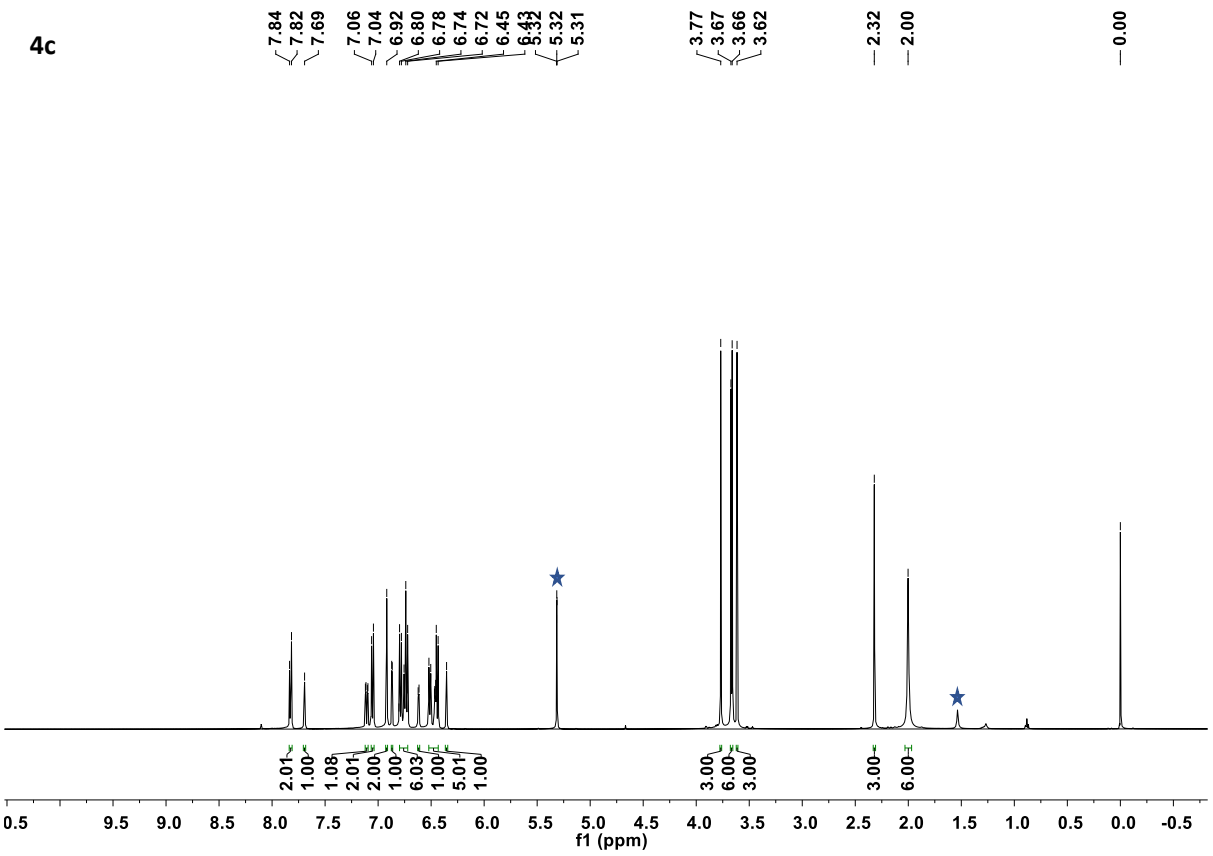


Fig S13 ^{1}H NMR spectra of the BODIPY **4c** (400 MHz, CD_2Cl_2).

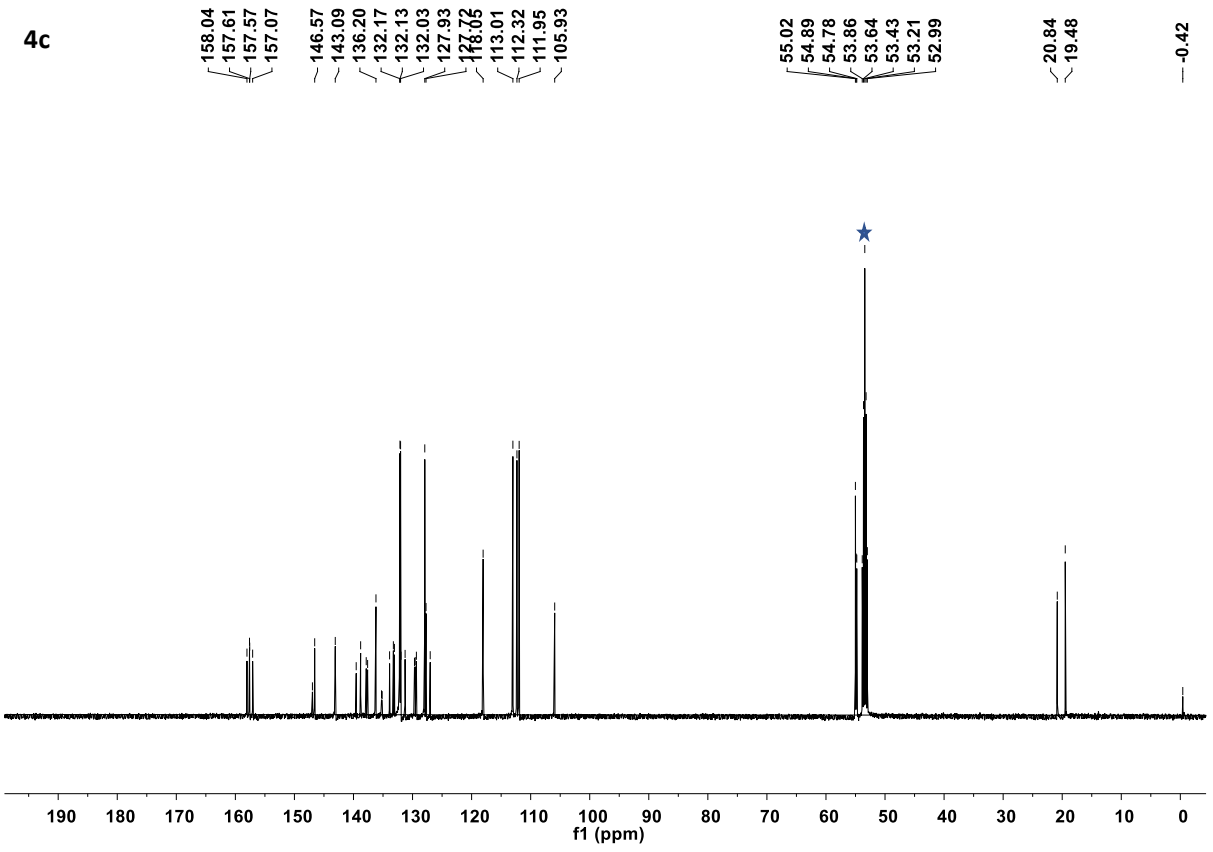


Fig S14 ^{13}C NMR spectra of the BODIPY **4c** (125 MHz, CD_2Cl_2).

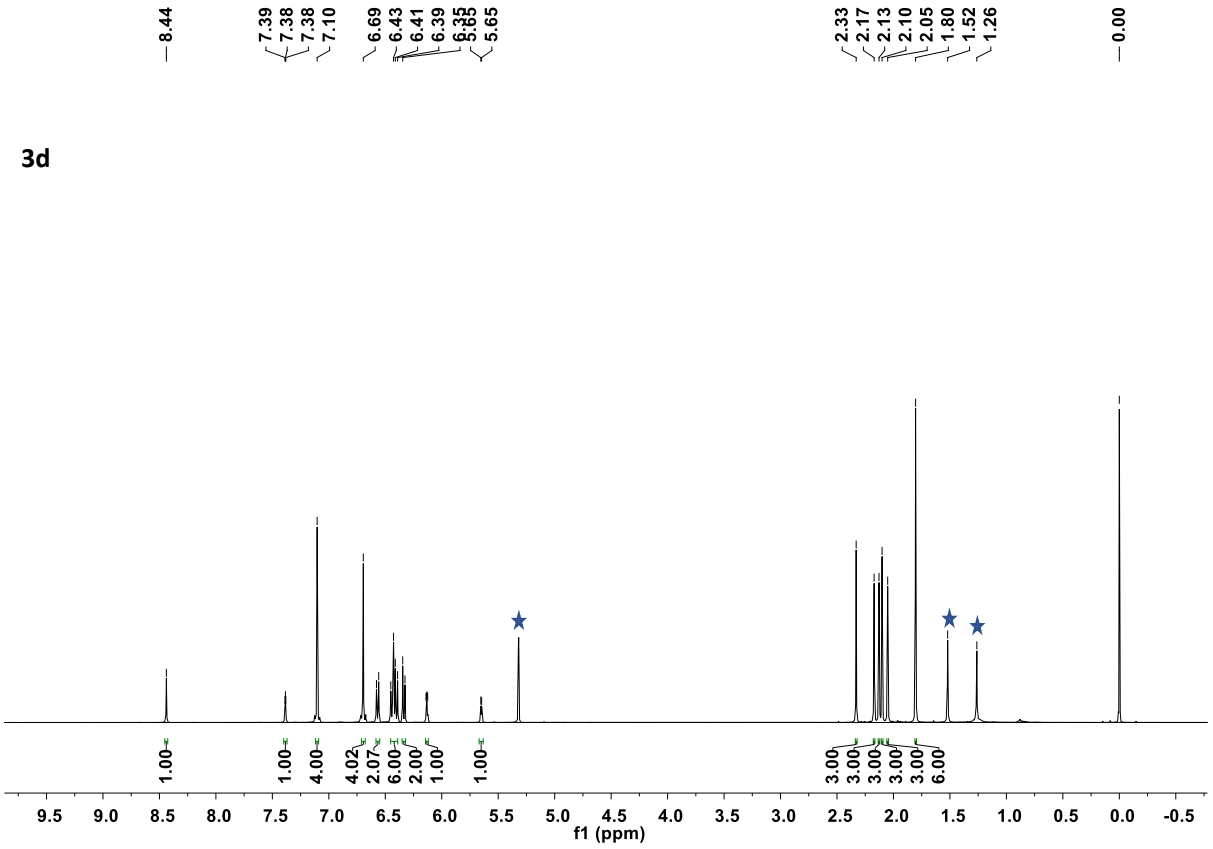


Fig S15 ^{1}H NMR spectra of the BODIPY **3d** (400 MHz, CD_2Cl_2).

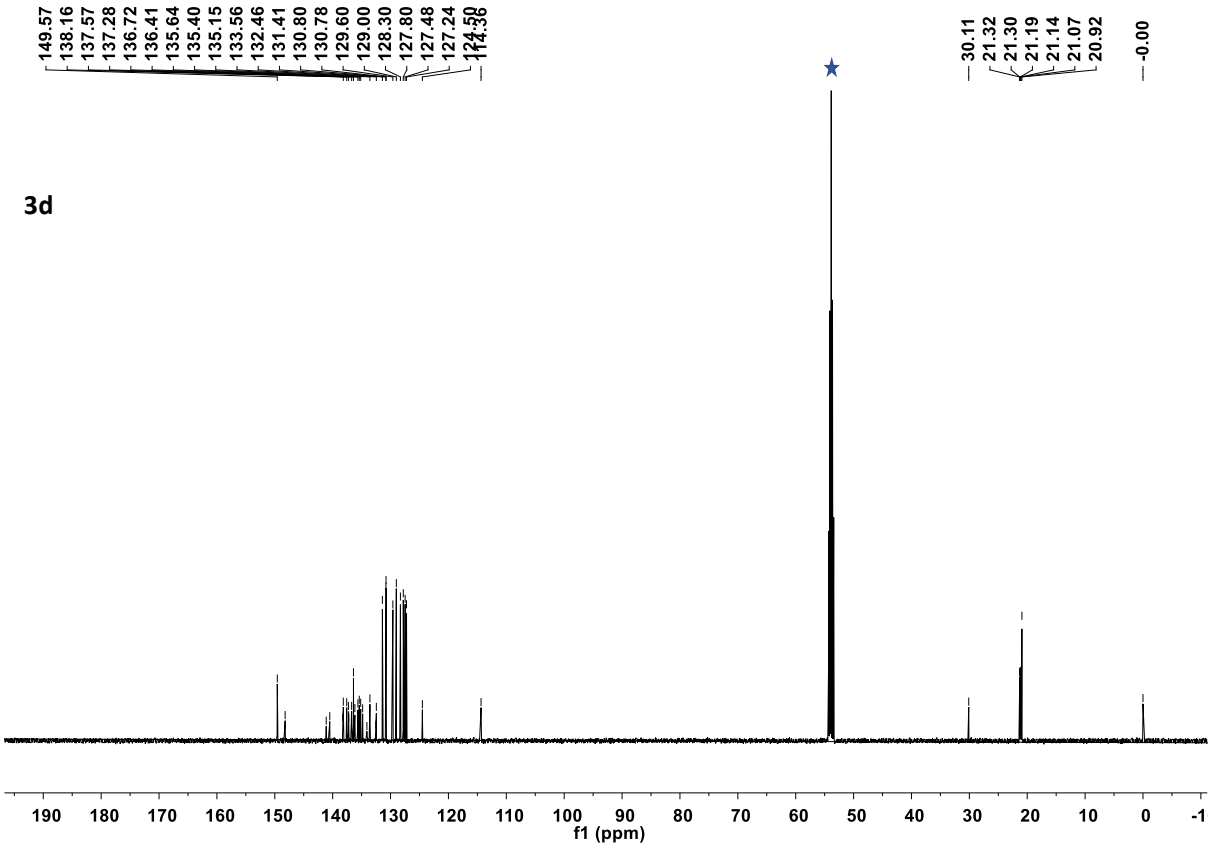


Fig S16 ^{13}C NMR spectra of the BODIPY **3d** (125 MHz, CD_2Cl_2).

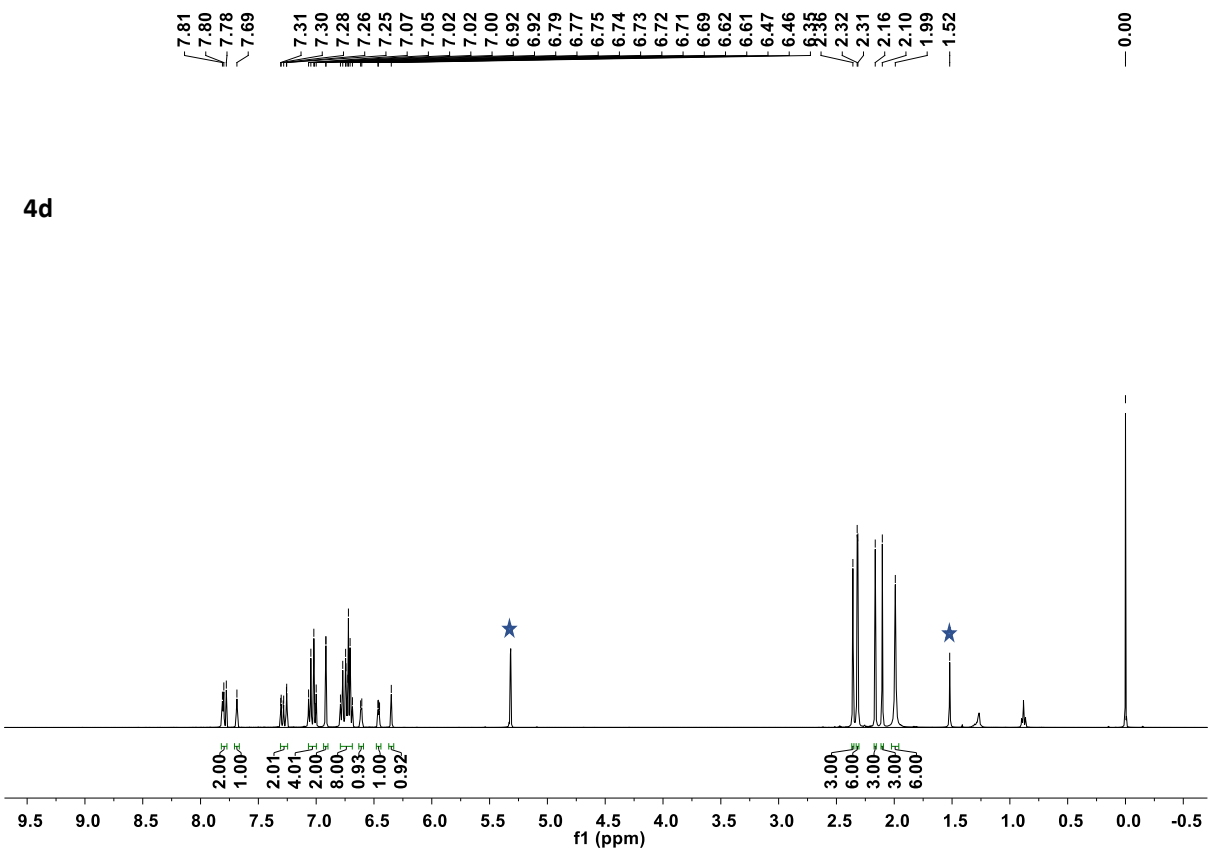


Fig S17 ^{1}H NMR spectra of the BODIPY **4d** (400 MHz, CD_2Cl_2).

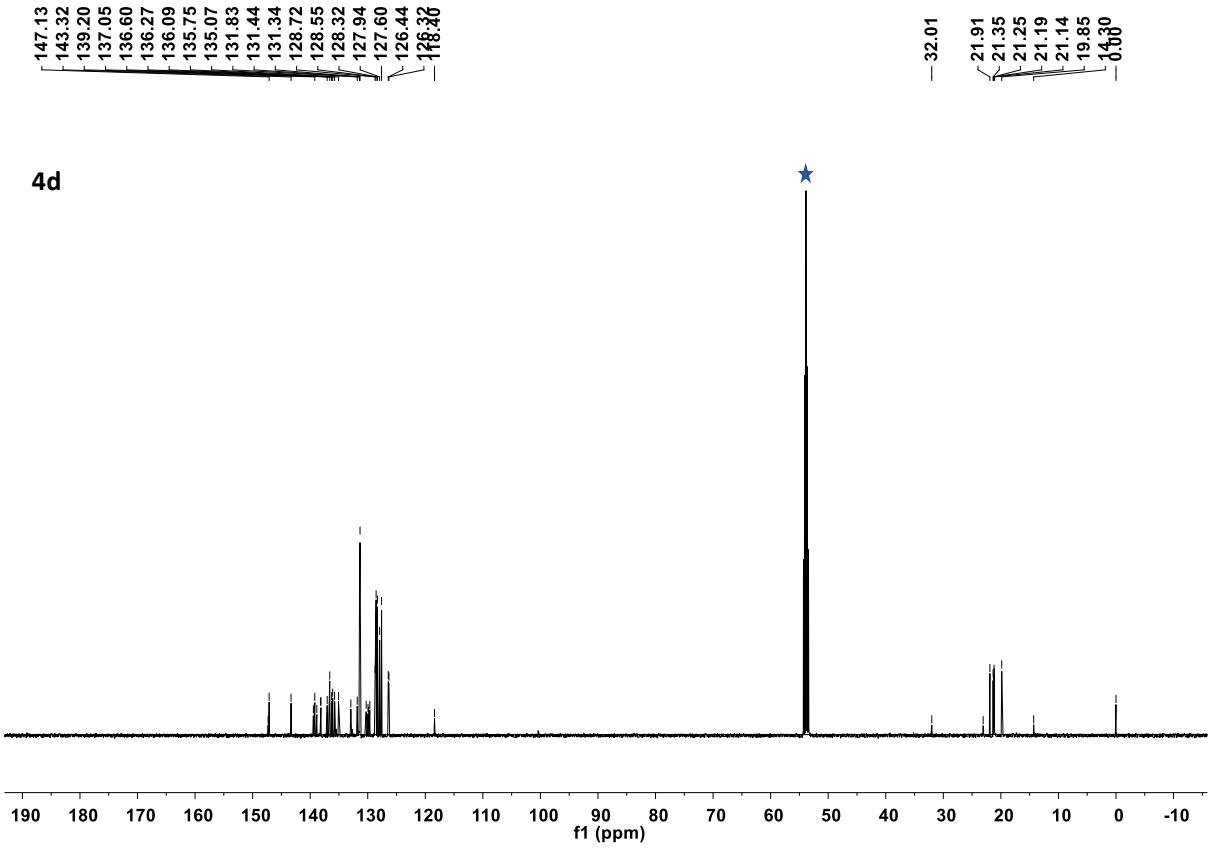


Fig S18 ^{13}C NMR spectra of the BODIPY **4d** (125 MHz, CD_2Cl_2).

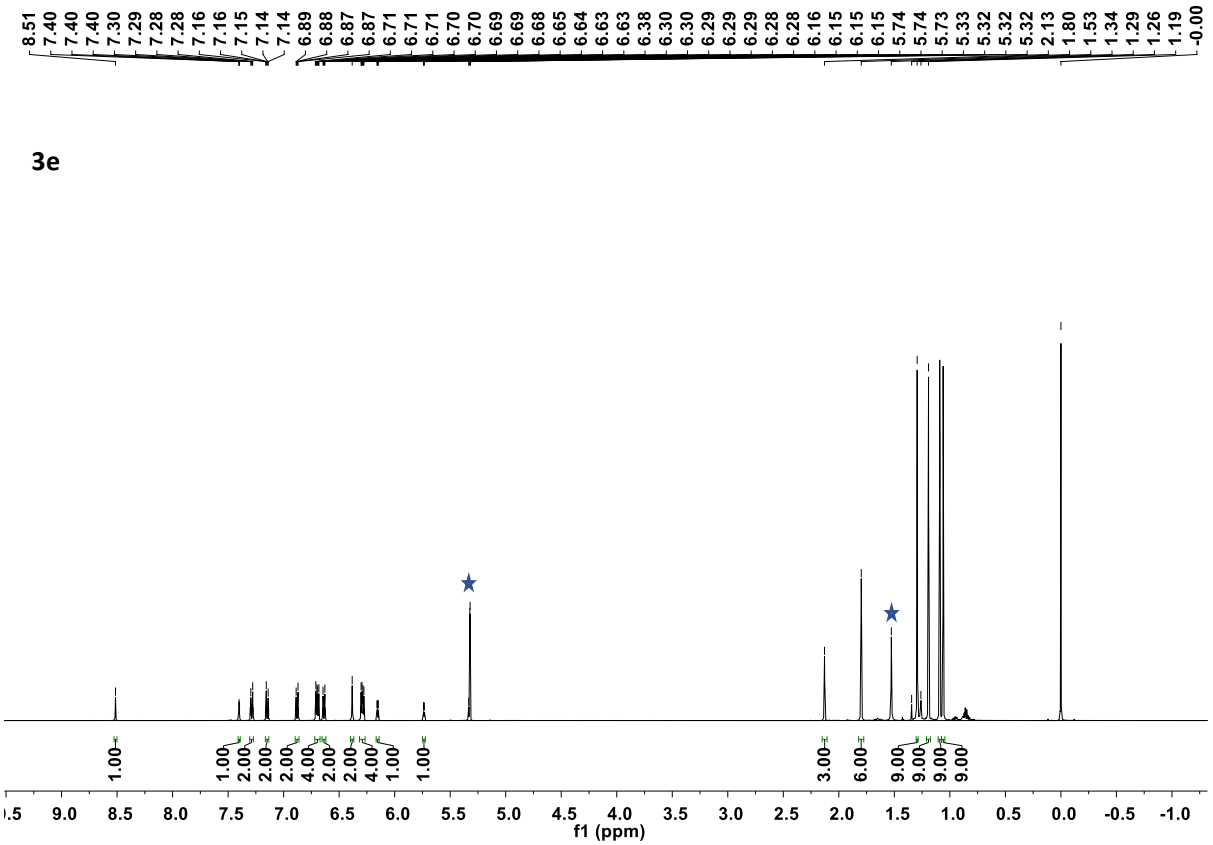


Fig S19 ^{1}H NMR spectra of the BODIPY **3e** (500 MHz, CD_2Cl_2).

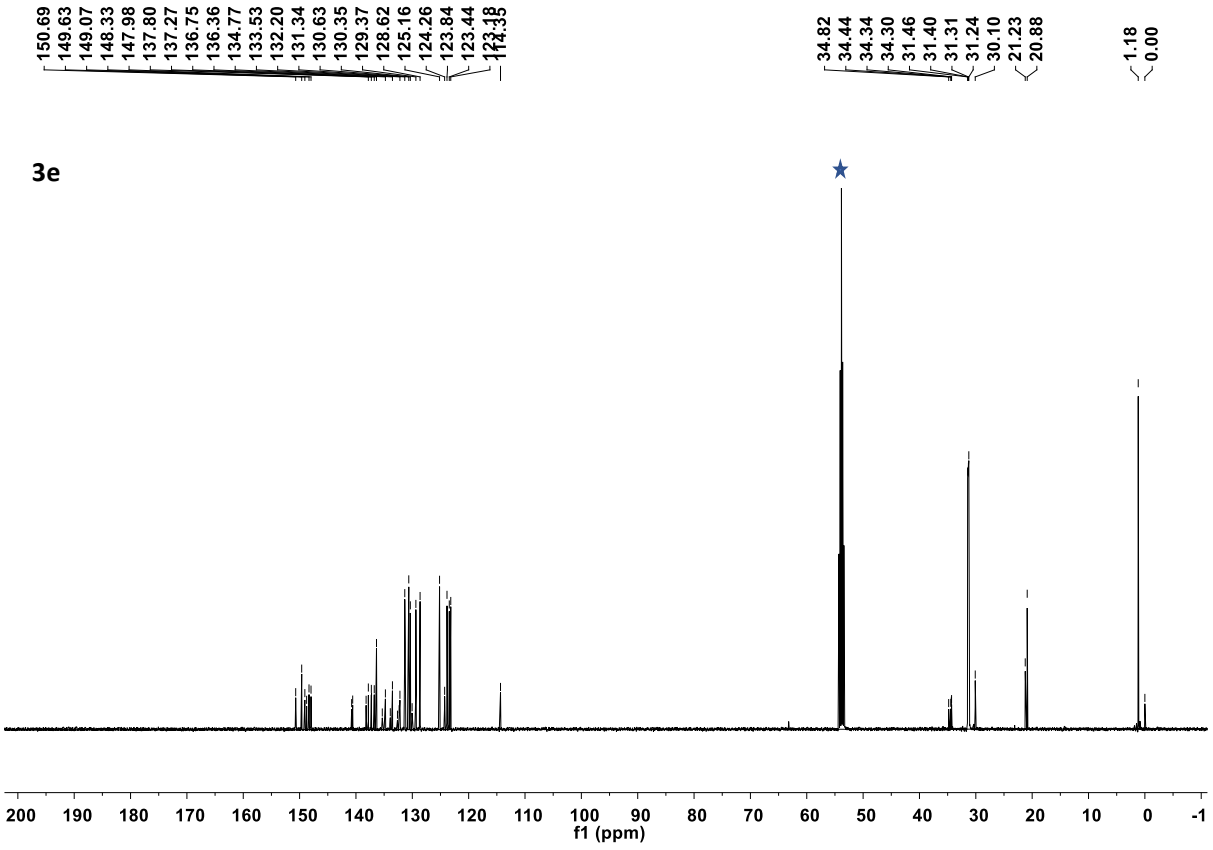


Fig S20^{13}C NMR spectra of the BODIPY **3e** (125 MHz, CD_2Cl_2).

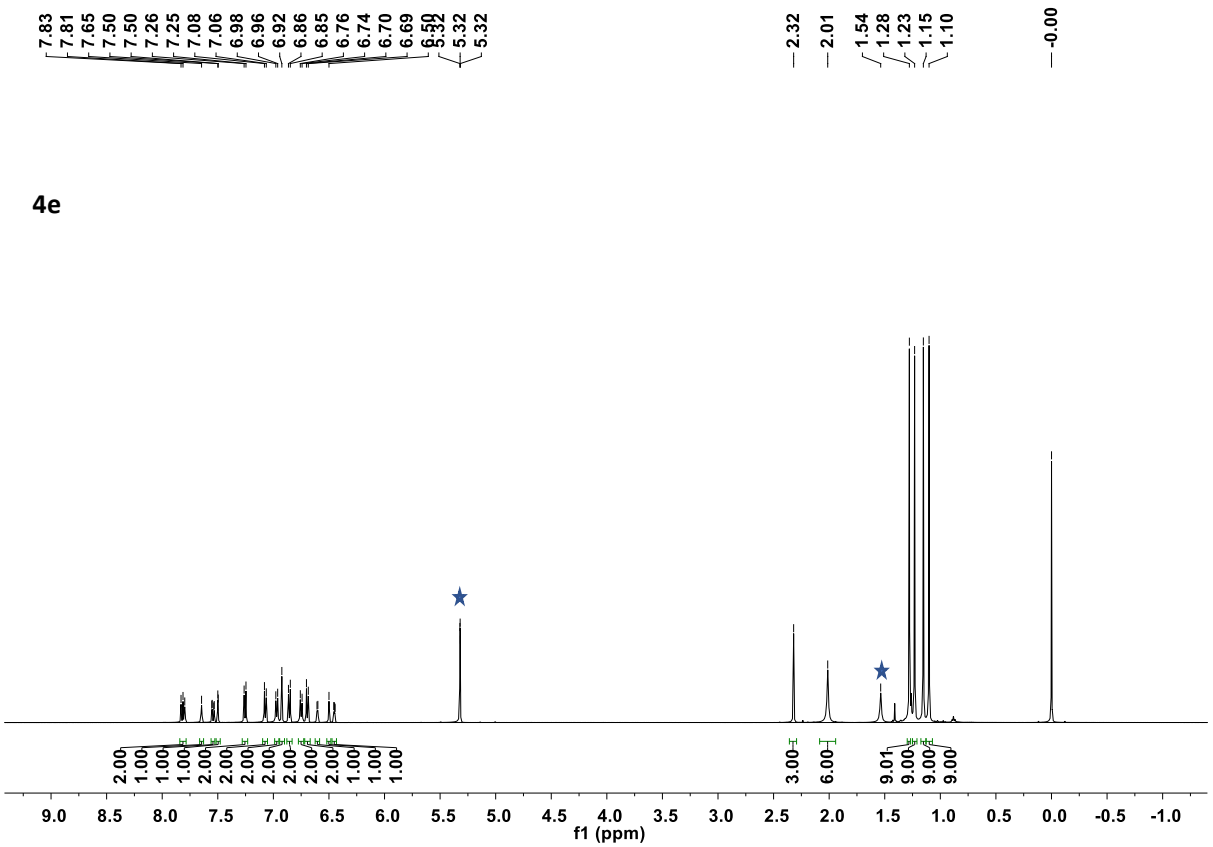


Fig S21 ^{1}H NMR spectra of the BODIPY **4e** (500 MHz, CD_2Cl_2).

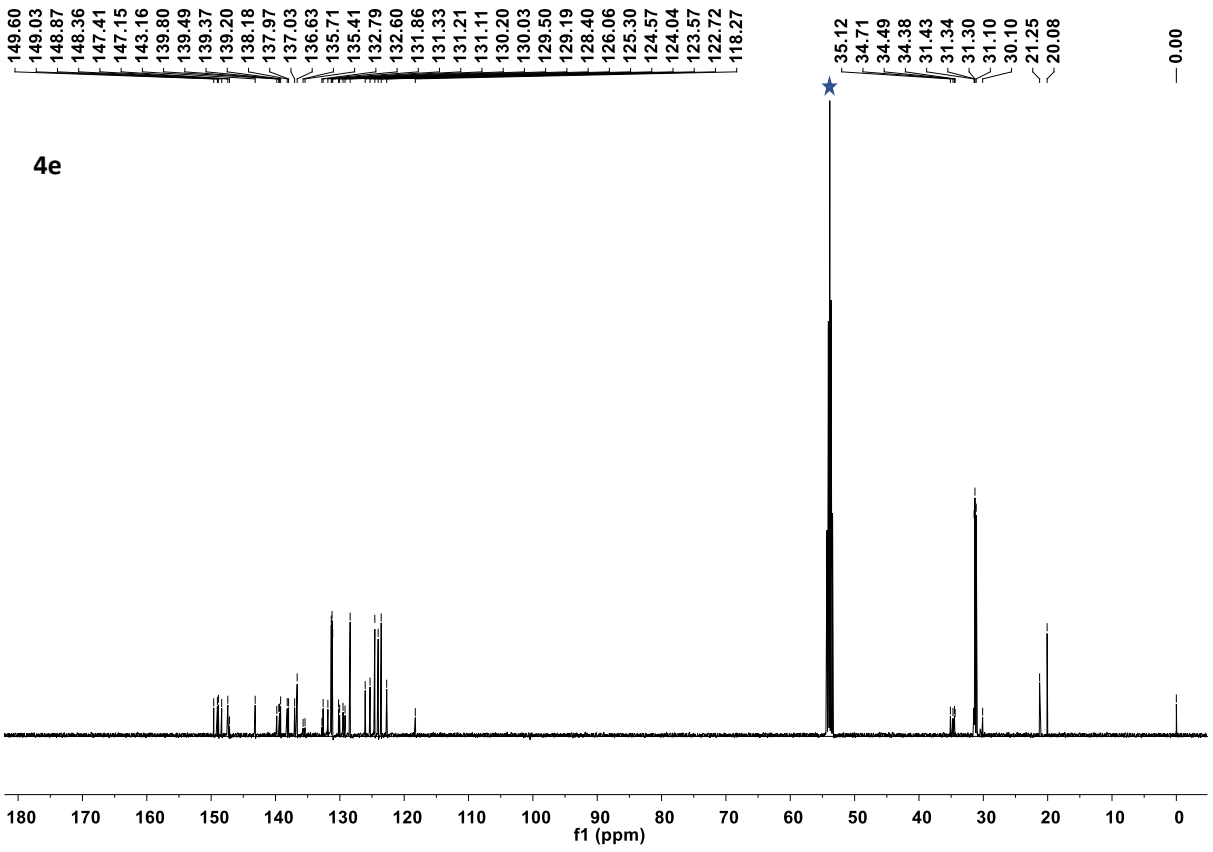


Fig S22 ^{13}C NMR spectra of the BODIPY **4e** (125 MHz, CD_2Cl_2).

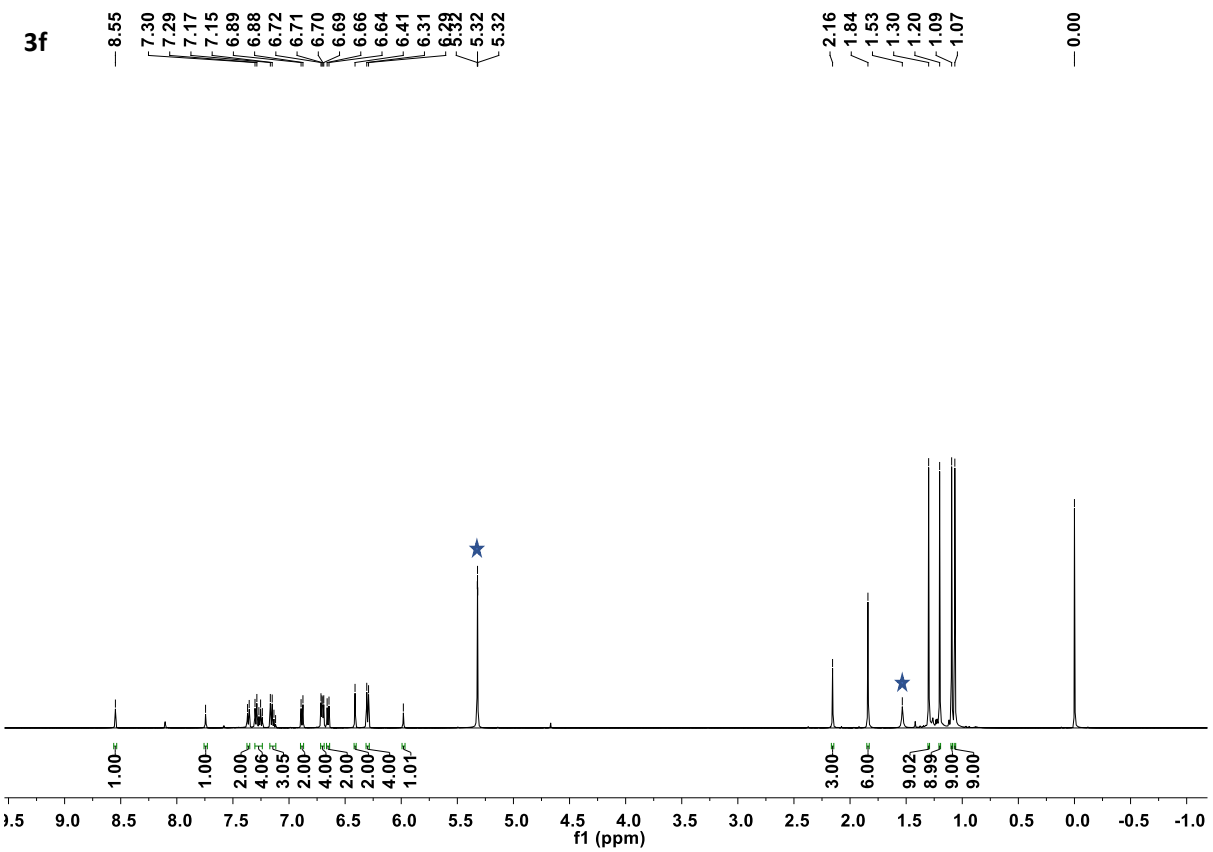


Fig S23 ^{1}H NMR spectra of the BODIPY **3f** (500 MHz, CD_2Cl_2).

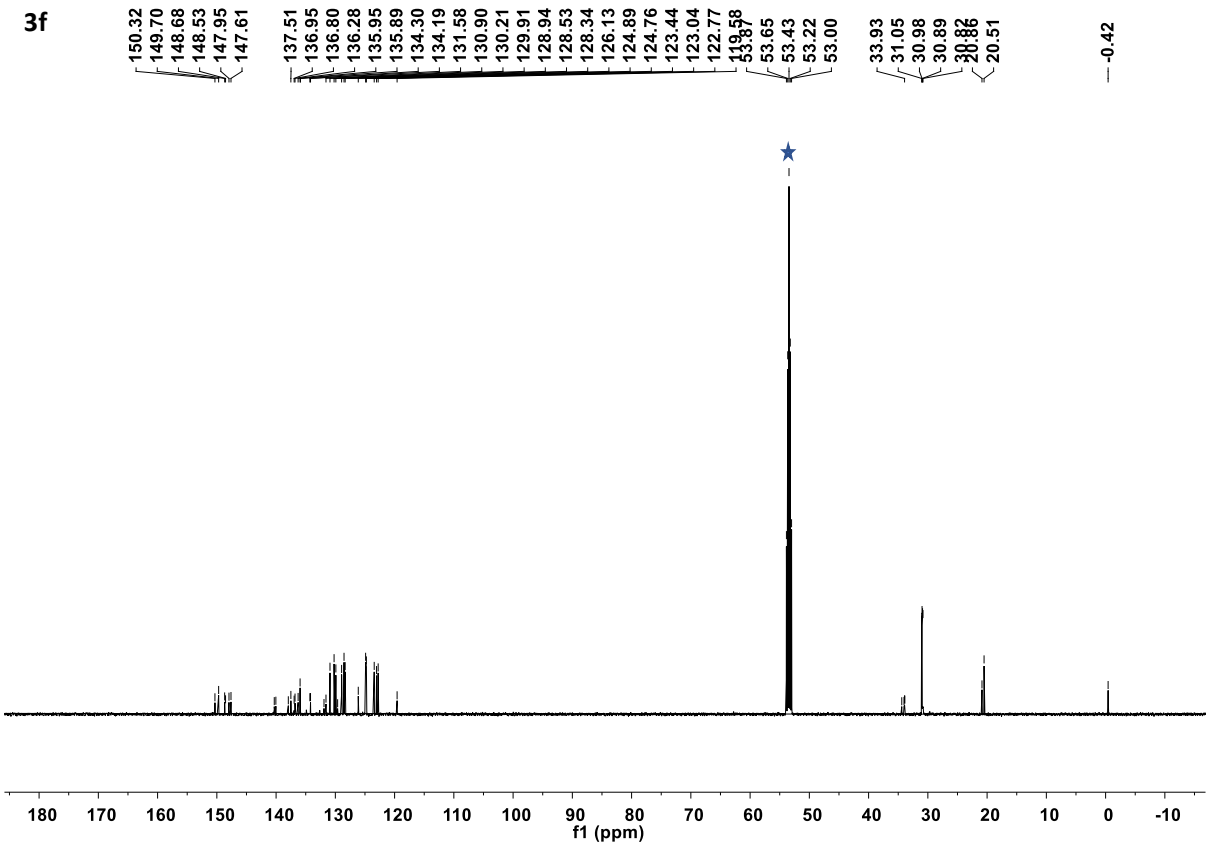


Fig S24 ^{13}C NMR spectra of the BODIPY **3f** (125 MHz, CD_2Cl_2).

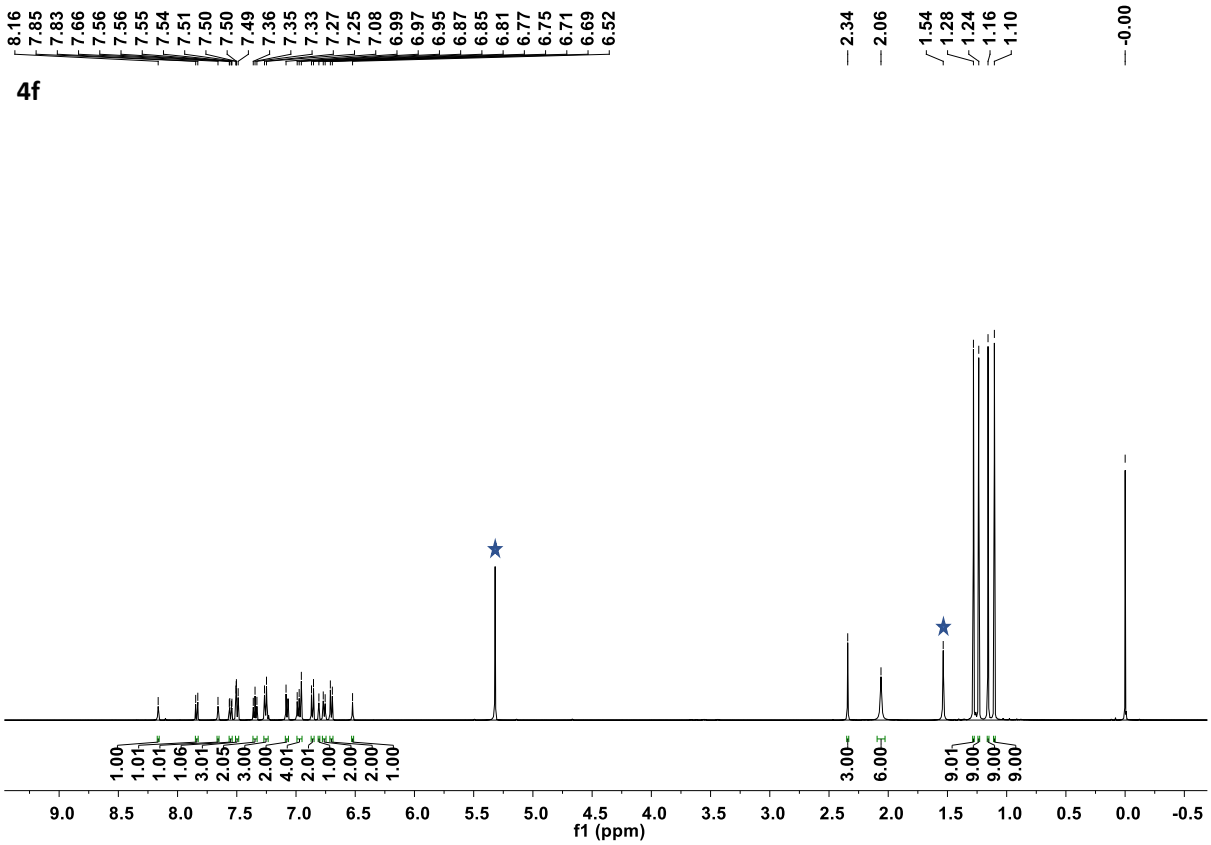


Fig S25 ^{1}H NMR spectra of the BODIPY **4f** (500 MHz, CD_2Cl_2).

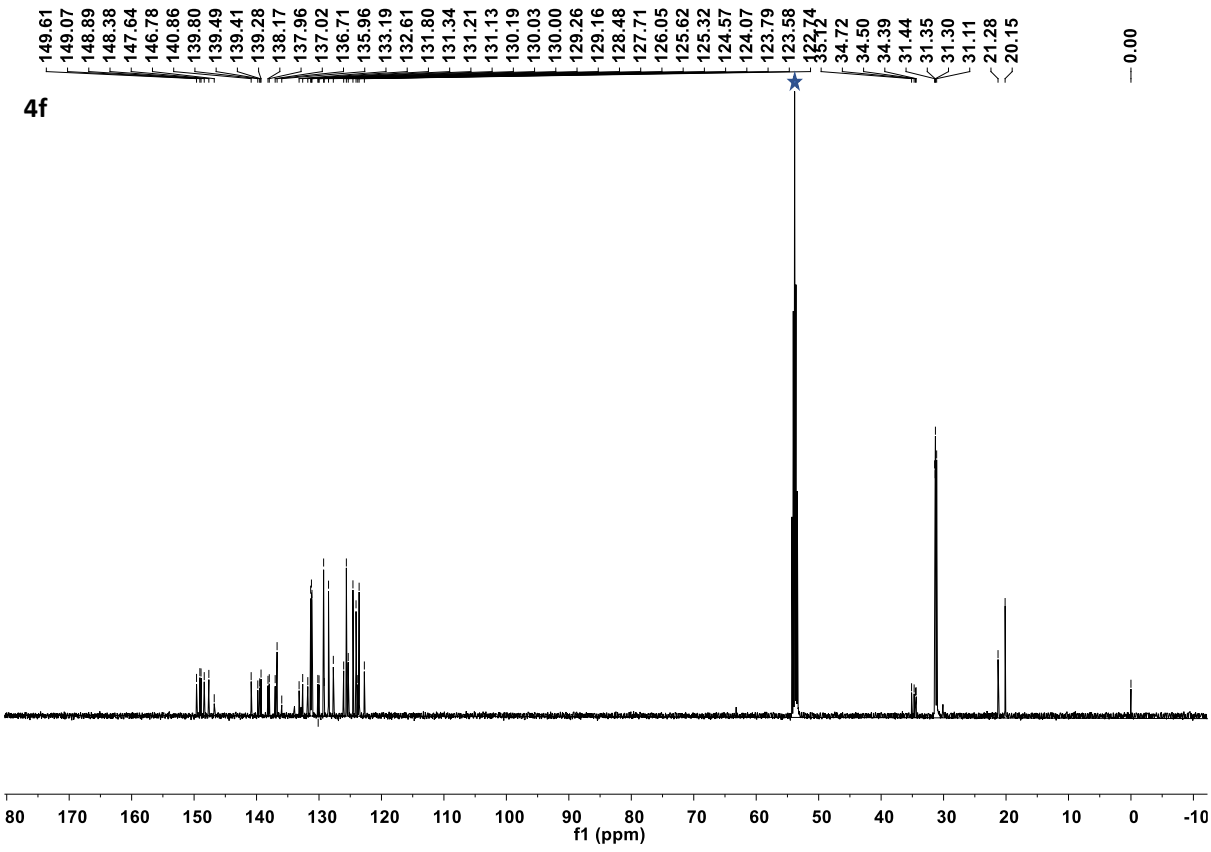
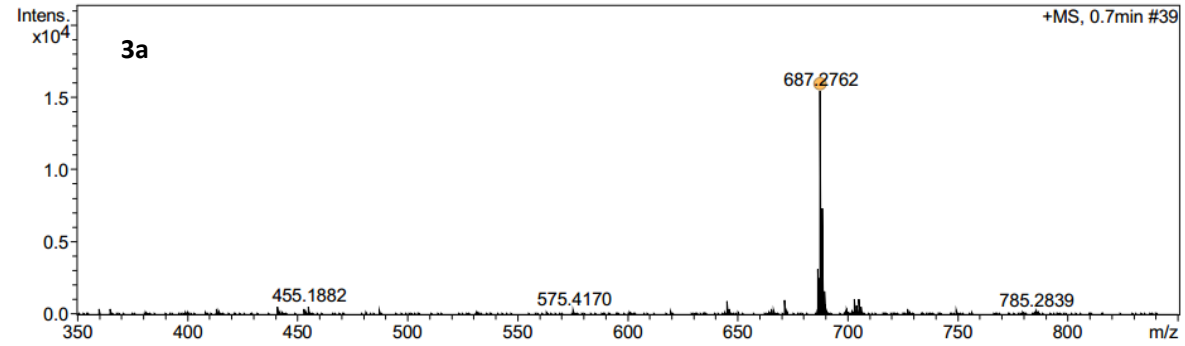


Fig S26 ^{13}C NMR spectra of the BODIPY **4f** (125 MHz, CD_2Cl_2).

Acquisition Parameter

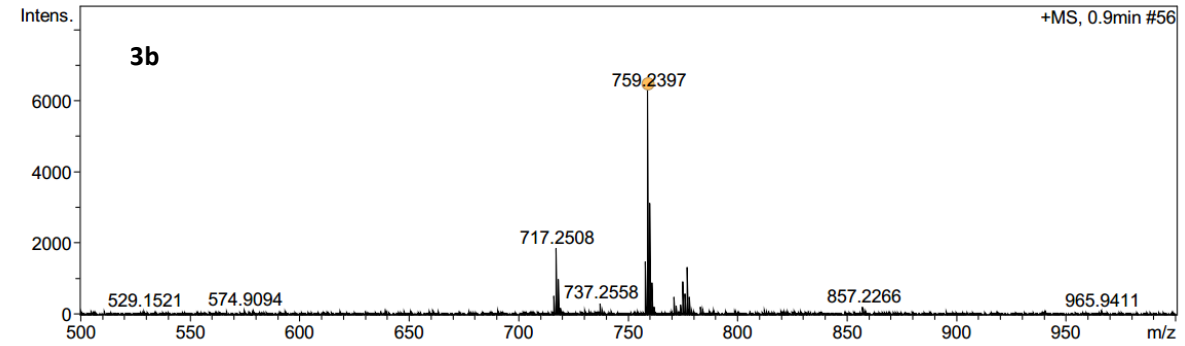
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	300 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1200 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
687.2762	1	C46H35BF2N2Na	687.2761	-0.1	8.6	1	100.00	29.5	even	ok

Acquisition Parameter

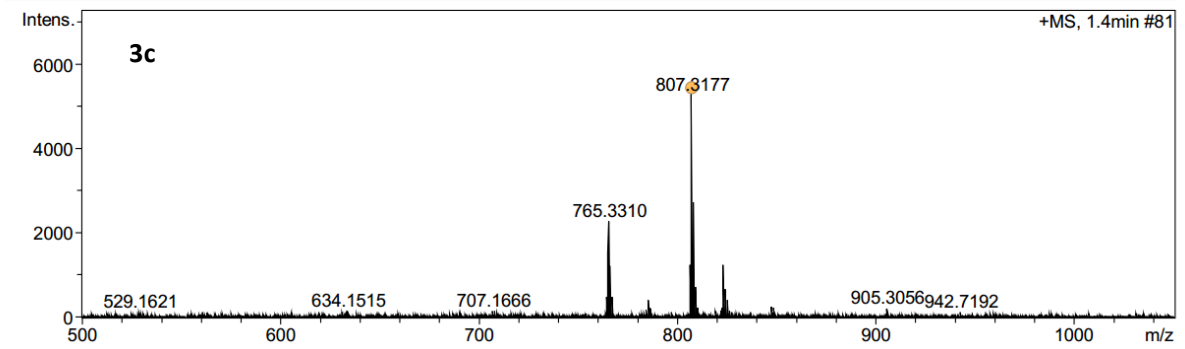
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	300 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1200 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
759.2397	1	C46H31BF6N2Na	759.2384	1.6	17.9	1	100.00	29.5	even	ok

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	300 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1200 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
807.3177	1	C50H43BF2N2NaO4	807.3185	-0.9	11.1	1	100.00	29.5	even	ok

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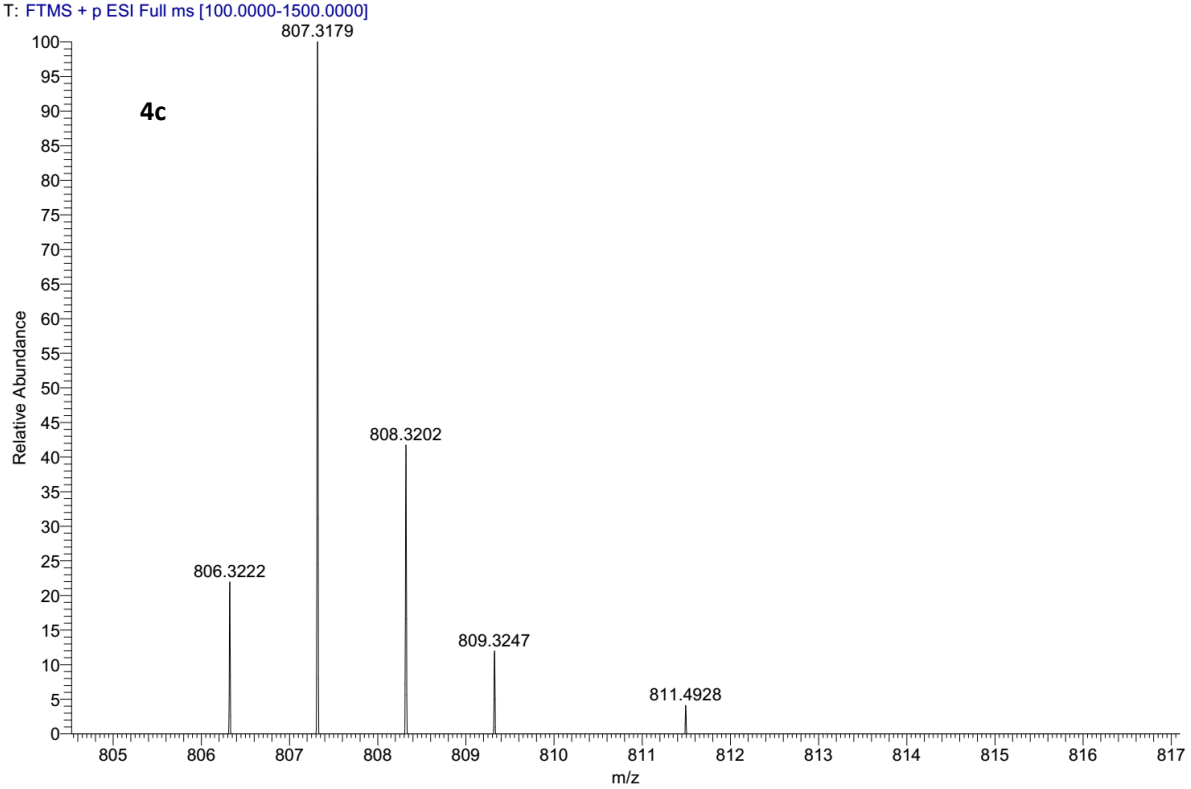

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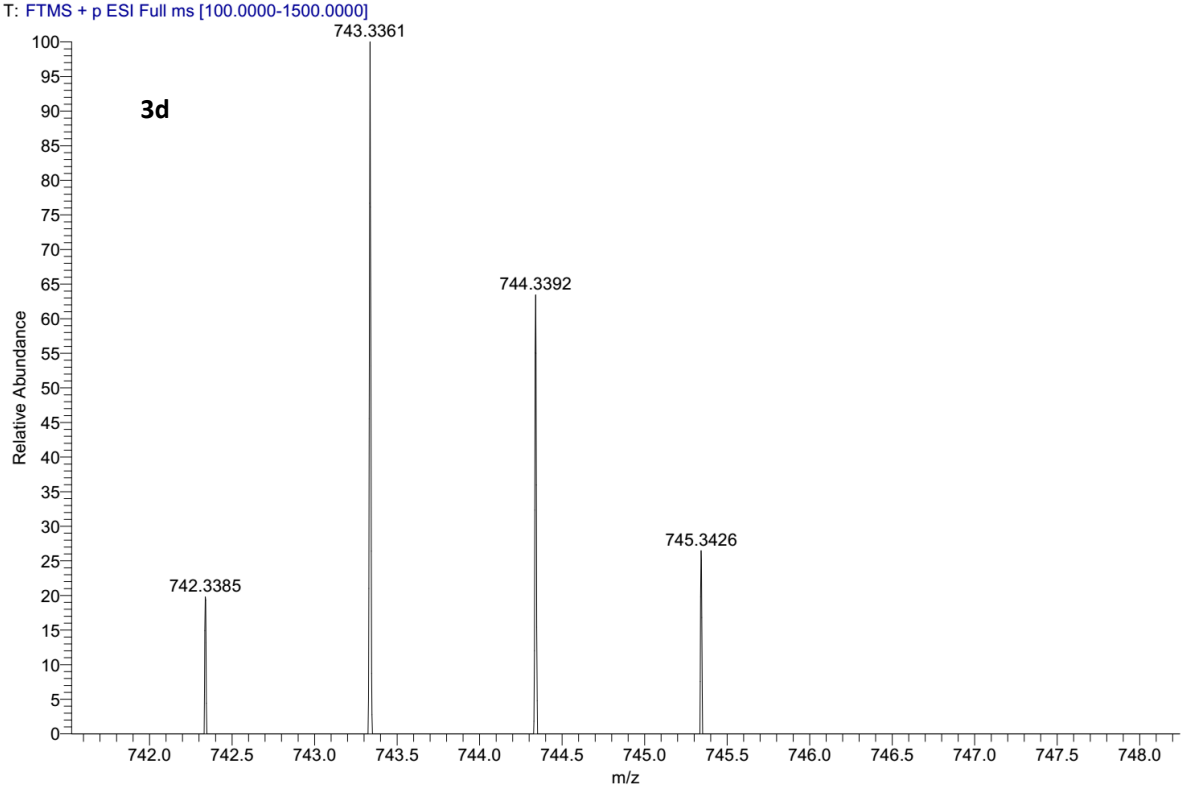

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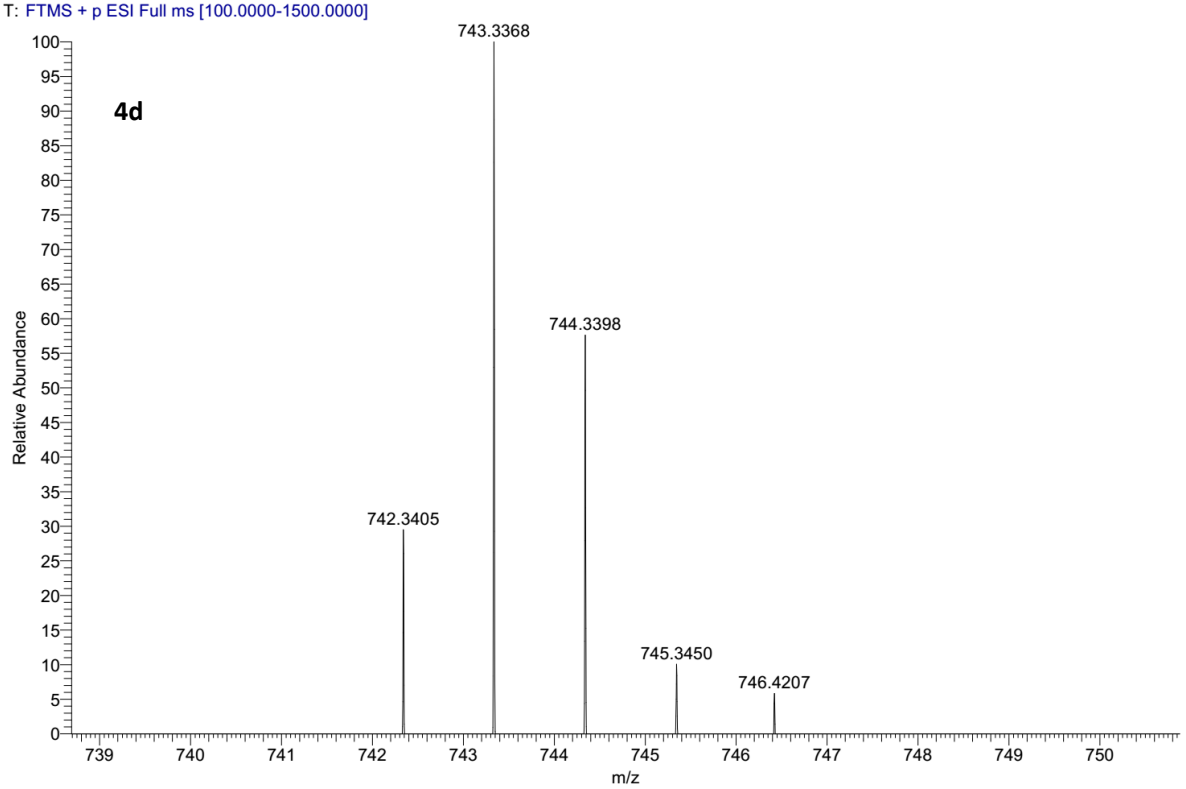

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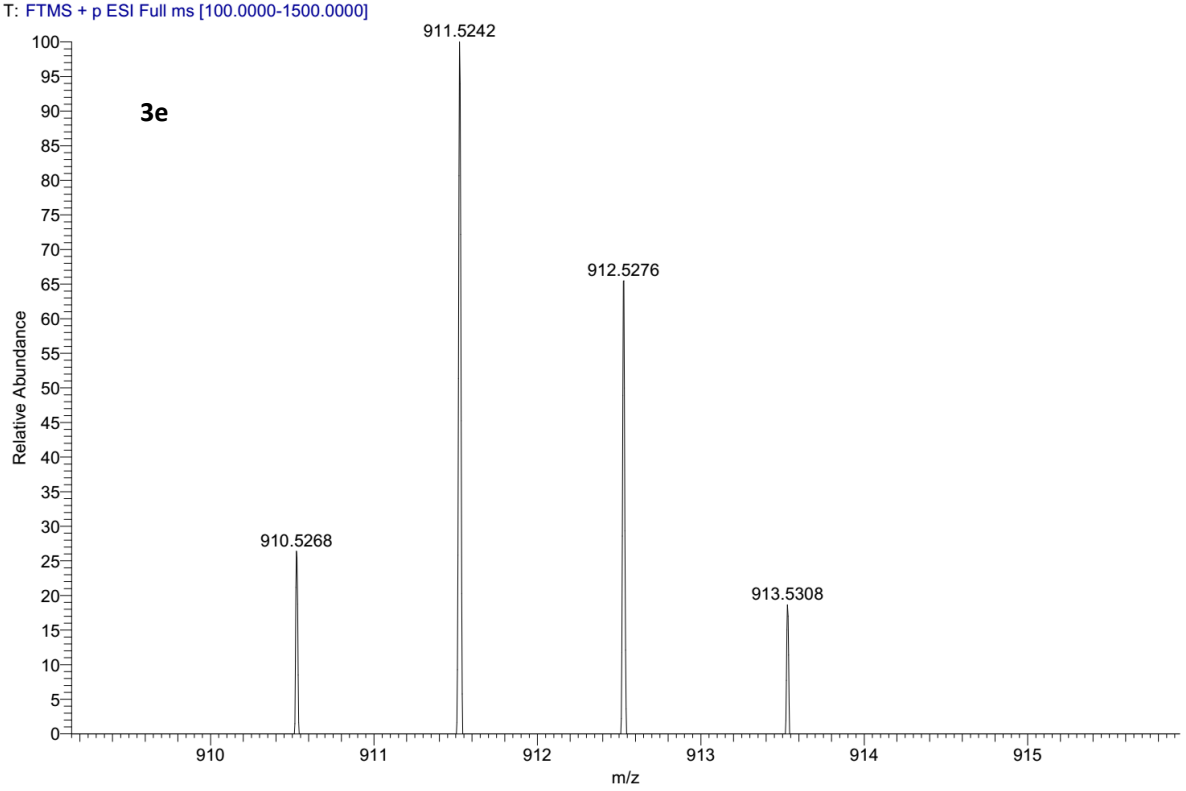

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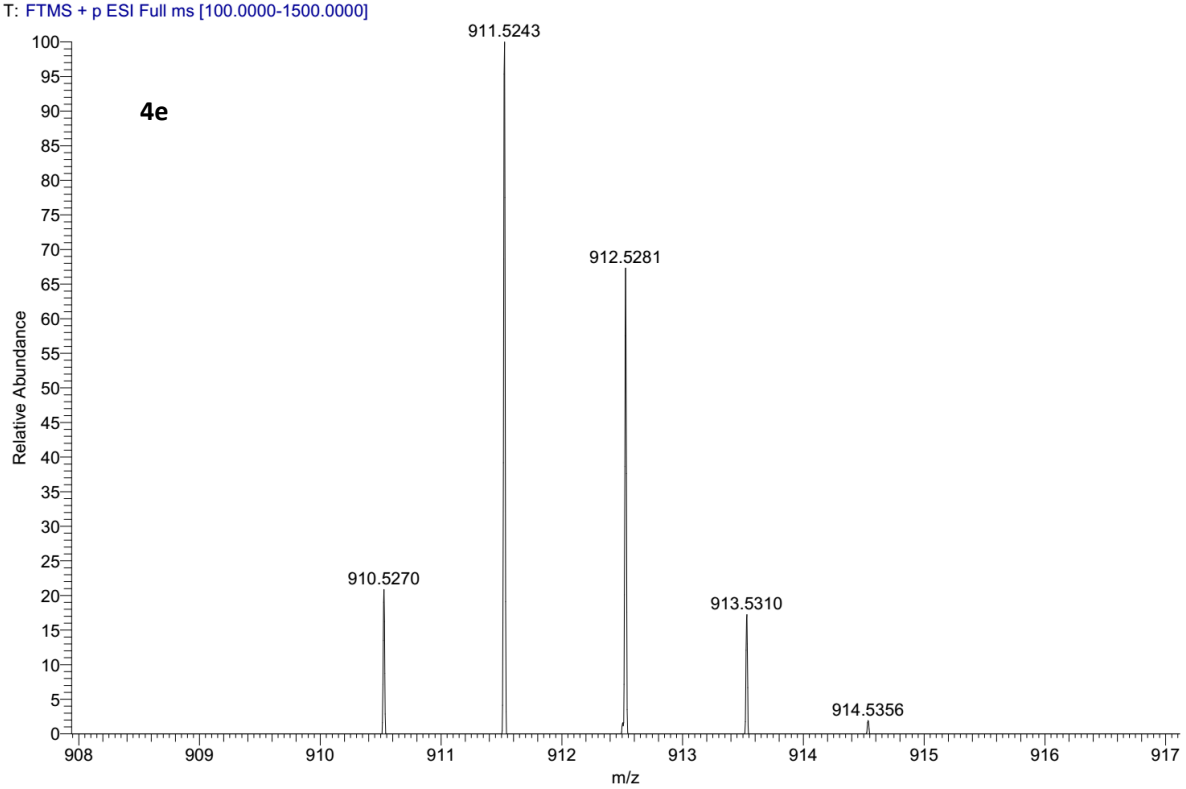
T: FTMS + p ESI Full ms [100.0000-1500.0000]



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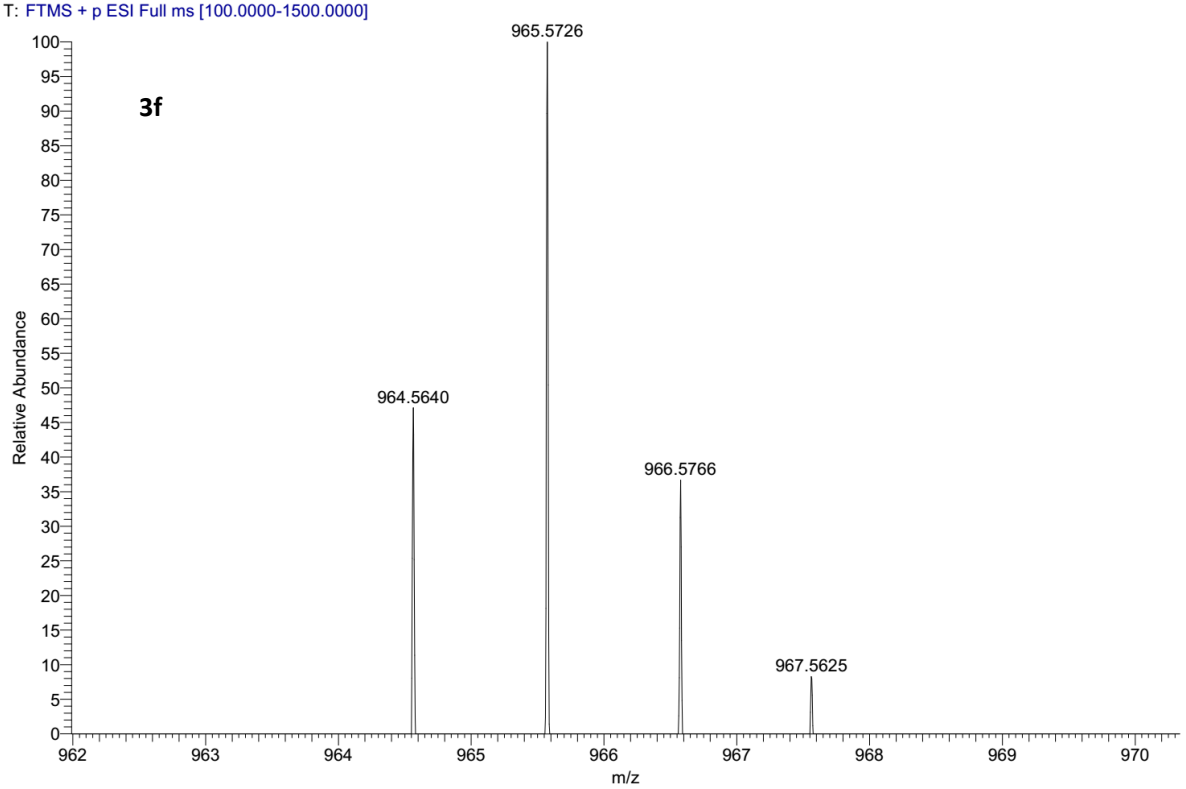
1f #13-22 RT: 0.12-0.21 AV: 10 NL: 4.80E4
T: FTMS + p ESI Full ms [100.0000-1500.0000]



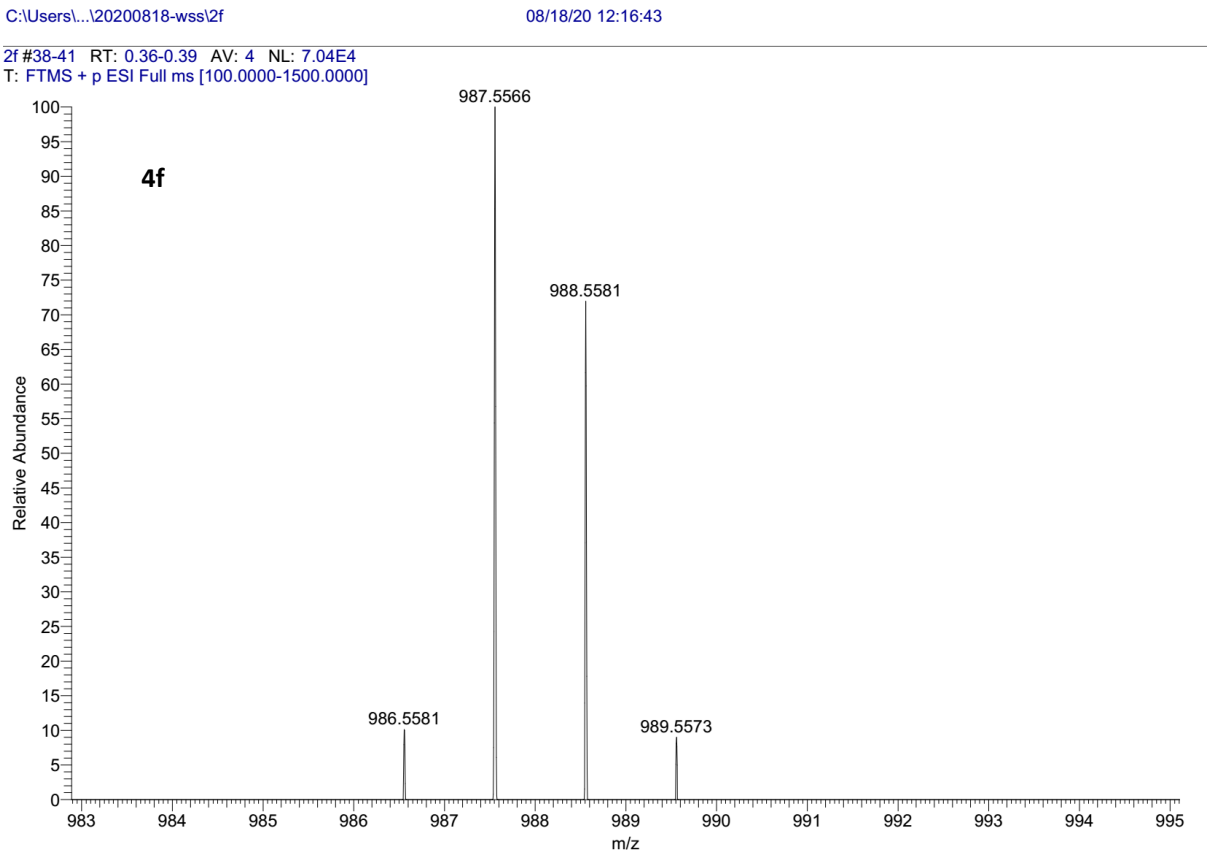


Fig S9. The HR-MS spectrum of **3a**-**3f** and **4c**-**4f**.

III. References

S1 C. L. Picou, E. D. Stevens, M. Shah and J. H. Boyer, Acta Crystallogr. Sect. C 1990, 46, 1148.

S2 SMART, SAINT, SADABS and SHELXTL, Bruker AXS Inc., Madison, 2000.

S3 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. J. Bearpark, J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, N. J. 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, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian 09, Revision B.01, Gaussian, Inc., Wallingford, CT, 2009.