Supporting Information for

Red Fluorescent BODIPY-Based Nanoparticles for Targeted Cancer Imaging-Guided Photodynamic Therapy

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S1. Synthesis and characterization of LaB-*X* compounds

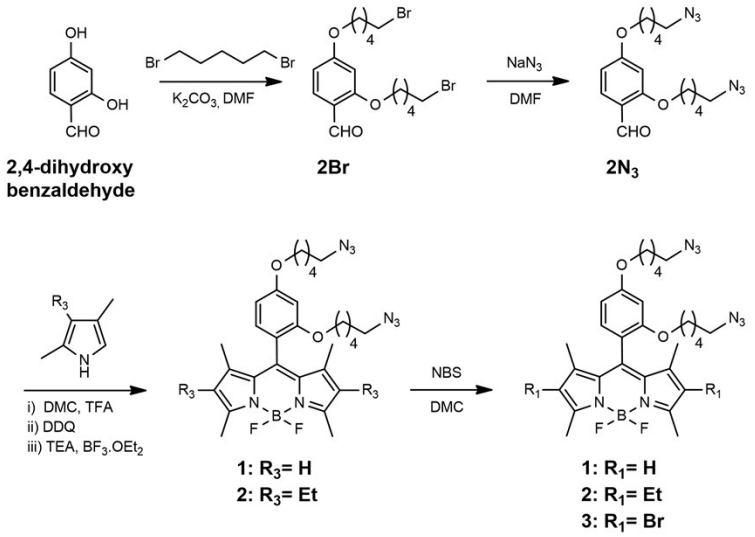

Figure S1. Preparation of BODIPY precursors and **1a**–**c**.

Compound 2Br. 2,4-dihydroxybenzaldehyde (2 g, 14.48 mmol), 1,5-dibromopentane (13.31 g, 57.92 mmol), and K_2CO_3 (8 g, 57.92 mmol) were added into DMF (30 mL). The mixture was stirred under argon atmosphere (90 ºC, overnight). After the reaction was completed, the mixture was extracted by EA/water, dried by $MgSO_4$, and the solvent was evaporated in vacuo. The resulting crude product was purified by silica gel column chromatography (Hx/EA = 5/1, v/v) to yield compound **2Br** as a yellow oil (3.7 g, 60.5% yield). ^{1}H NMR (300 MHz, $CDCl_3$): δ 10.33 (s, 1H), 7.82-7.79 (d, 1H), 6.54-6.51 (d, 1H), 6.43 (s, 1H), 4.08-4.04 (q, 4H), 3.47-3.43 (t, 4H), 1.97-1.86 (m, 8H), 1.69-1.65 (m, 8H).

Compound $2N_3$. Compound **2Br** (3.45 g, 7.9 mmol) and NaN_3 (15.4 g, 237 mmol) were added into DMF (50 mL). The mixture was stirred under argon atmosphere (2 days, RT). After the reaction was completed, the mixture was extracted by EA/water, dried by anhydrous $MgSO_4$, and the solvent was evaporated in vacuo. The resulting crude product was purified by silica gel column chromatography (Hx/EA = 3/1, v/v) to yield a brown oil **$2N_3$** (2.42 g, 85 % yield). ^{1}H NMR (300 MHz, $CDCl_3$): δ 10.32 (s, 1H), 7.82-7.79 (d, 1H), 6.53-6.51 (d, 1H), 6.43 (s, 1H), 4.08-4.03 (q, 4H), 3.35-3.3 (t, 4H), 1.91-1.82 (m, 4H), 1.69-1.67 (m, 4H), 1.59-1.56 (m, 4H).

BODIPY 1a. BODIPY **1a** was synthesized according to the reported recipe.[1] Briefly, 2,4-dimethyl pyrrole (0.6 g, 6.3 mmol) and compound **$2N_3$** (1.14 g, 3.15 mmol) were dissolved in 100 mL of dried CH_2Cl_2 containing a few droplets of TFA at room temperature under argon atmosphere. The DDQ (0.72 g, 3.15 mmol) was added to the mixture, followed by addition of TEA (2 mL) and $BF_3{\cdot}Et_2O$ (2.5 mL). BODIPY

1a was afforded by column chromatography as a bright orange solid (0.46 g, 25.3 % yield). ^{1}H-NMR (300 MHz, $CDCl_3$, δ, ppm): δ 7.01-6.98 (d, 1H), 6.59-6.56 (d, 1H), 6.53 (s, 1H), 5.96 (s, 2H), 4.03-3.99 (t, 2H), 3.95-3.91 (t, 2H), 3.36-3.32 (t, 2H), 3.11-3.06 (t, 2H), 2.55 (s, 6H), 1.88-1.83 (m, 2H), 1.73-1.60 (m, 6H), 1.5 (s, 6H), 1.28-1.23 (m, 2H).

BODIPY 1b. The synthetic procedures of BODIPY **1b** was same as that of BODIPY **1a** except the replacement of 2,4-dimethyl pyrrole with 3-ethyl-2,4-dimethyl pyrrole. BODIPY **1b** was gained as a orange solid (0.49 g, 32% yield). ^{1}H-NMR (300 MHz, $CDCl_3$, δ, ppm): δ 7.0-6.97 (d, 1H), 6.58-6.56 (d, 1H), 6.52 (s, 1H), 4.04-3.99 (t, 2H), 3.94-3.90 (t, 2H), 3.36-3.31 (t, 2H), 3.08-3.04 (t, 2H), 2.52 (s, 6H), 2.32-2.30 (q, 4H), 1.89-1.84 (m, 2H), 1.71-1.69 (m, 6H), 1.63-1.61 (m, 2H), 1.41 (s, 6H), 1.27-1.24 (m, 2H), 1.01-0.96 (t, 6H).

BODIPY 1c. BODIPY **1a** (0.3 g, 0.52 mmol) was dissolved in dried CH_2Cl_2, followed by the addition of N-bromosuccinimide (NBS) (0.23 g, 1.3 mmol). After substitution by argon air, the mixture was stirred at room temperature for overnight. After the removal of the solvent, BODIPY **1c** was afforded by column chromatography as a red solid (0.316 g, 82.7% yield). ^{1}H NMR (300MHz, $CDCl_3$, δ, ppm): δ 6.96-6.94 (d, 1H), 6.61-6.58 (d, 1H), 6.54 (s, 1H), 4.05-4.0 (t, 2H), 3.94-3.90 (t, 2H), 3.37-3.33 (t, 2H), 3.12-3.07 (t, 2H), 2.64 (s, 6H), 1.89-1.85 (m, 2H), 1.72-1.64 (m, 6H), 1.52 (s, 6H), 1.45-1.41 (m, 2H), 1.25-1.18 (m, 2H).

BODIPY 2a–2c. BODIPY **2a** and **2b** were prepared following the same synthetic recipe. A representative procedure is described for BODIPY **2a**.

BODIPY **1a** (118 mg, 0.2 mmol) and benzaldehyde (76 mg, 0.7 mmol) were dissolved in dry DMF (10 mL), followed by the addition of acetic acid (1 mL) and piperidine (1 mL). The mixture was heated for 4 h at 130 ºC under argon atmosphere and then the solvent was removed by a rotary evaporator. The resulting crude product was purified by column chromatography (CH_2Cl_2/Hx = 1/1, v/v) to yield BODIPY **2a** as a black blue solid (94 mg, 61% yield). ^{1}H NMR (300 MHz, $CDCl_3$, δ, ppm): δ 7.78-7.72 (d, 2H), 7.65-7.63 (d, 4H), 7.43-7.38 (m, 4H), 7.34-7.32 (d, 2H), 7.28-7.26 (d, 1H), 7.23 (s, 1H), 7.04-7.02 (d, 1H), 6.64-6.55 (m, 4H), 4.05-4.0 (t, 2H), 3.96-3.92 (t, 2H), 3.37-3.32 (t, 2H), 3.10-3.05 (t, 2H), 1.89-1.85 (m, 2H), 1.71-1.67 (m, 5H), 1.65 (s, 6H), 1.45-1.43 (m, 2H), 1.27-1.23 (m, 3H). ^{13}C NMR (75.4 MHz, $CDCl_3$, δ, ppm): δ 161.47, 157.36, 152.22, 148.86, 142.02, 136.78, 135.93, 134.37, 130.41, 129.23, 127.67, 119.47, 117.49, 116.79, 105.71, 100.43, 68.36, 67.85, 51.36, 28.83, 28.22, 23.43, 23.25, 14.44.

BODIPY **2b** was prepared from BODIPY **1b** following the recipe described above to yield a black green solid (110 mg, 55% yield). ^{1}H NMR (300 MHz, $CDCl_3$, δ, ppm): δ 7.83-7.78 (d, 2H), 7.64-7.62 (d, 4H), 7.42-7.40 (m, 4H), 7.37-7.35 (d, 2H), 7.30-7.27 (d, 2H), 7.02-7.0 (d, 1H), 6.6-6.54 (m, 4H), 4.04-3.99 (t, 2H), 3.95-3.91 (t, 2H), 3.35-3.3 (t, 2H), 3.08-3.04 (t, 2H), 2.66-2.59 (q, 4H), 1.88-1.83 (m, 2H), 1.7-1.62 (m, 8H), 1.59 (s, 6H), 1.3-1.26 (m, 2H), 1.2-1.15 (m, 6H). ^{13}C NMR (75.4 MHz, $CDCl_3$, δ, ppm): δ 161.43, 157.54, 149.97, 138.93, 137.73, 136.58, 135.66, 133.98, 133.42, 130.53, 128.9, 128.61, 127.45, 126.46, 120.39, 117.64, 117.22, 105.96, 100.47, 68.5, 67.89, 50.62, 28.77, 28.46, 18.36, 14.88, 14.17, 11.17.

BODIPY **2c** was prepared according to the reported recipe with some minor modifications.[2] BODIPY **1c**

(238 mg, 0.32 mmol) and benzaldehyde (120 mg, 1.13 mmol) were refluxed overnight under argon atmosphere in a mixture of toluene (20 mL), acetic acid (1 mL), and piperidine (1.2 mL) and then the solvent was removed under reduced pressure. The resulting crude product was purified by silica gel column chromatography (CH_2Cl_2/Hx = 1.5/1, v/v). The green colored fraction was collected and the residual solvent was removed under reduced pressure to yield BODIPY **2c** (109 mg, 37% yield). ^{1}H NMR (300 MHz, $CDCl_3$, δ, ppm): δ 8.16-8.11 (d, 2H), 7.77-7.66 (d, 6H), 7.43-7.35 (m, 6H), 7.01-6.98 (d, 1H), 6.63-6.55 (m, 2H), 4.06-4.02 (t, 2H), 3.96-3.92 (t, 2H), 3.37-3.33 (t, 2H), 3.13-3.08 (t, 2H), 1.9-1.85 (m, 2H), 1.72-1.64 (m, 8H), 1.61 (s, 6H), 1.47-1.43 (m, 2H). ^{13}C NMR (75.4 MHz, $CDCl_3$, δ, ppm): δ 162.01, 157.28, 151.36, 148.08, 141.17, 139.22, 137.08, 133.13, 130.29, 129.41, 128.99, 127.89, 126.75, 118.34, 116.2, 106.12, 68.41, 68.13, 51.35, 28.73, 28.42, 23.47, 23.33, 13.48.

BODIPY 3a–3c. BODIPY **3a**–**3c** were prepared by the CuAAC click reaction following the recipe as in our reported literature.[3] A representative procedure is described for BODIPY **3a**.

BODIPY **2a** (55 mg, 0.16 mmol), lactose acetate propargyl (67 mg, 0.175 mmol), NaAsc (158 mg, 0.797 mmol), and $CuSO_4 \cdot 5H_2O$ (80 mg, 0.32 mmol) were dissolved in a mixture of THF/water (15/3 mL, v/v). The solution was stirred for 24 h at room temperature, extracted with EA/water, and dried over $MgSO_4$. The solvent was removed by a rotary evaporator and the resulting crude product was purified by silica gel column chromatography using EA/Hx to yield BODIPY **3a** as a black blue solid (60 mg, 52% yield). ^{1}H NMR (300 MHz, $CDCl_3$, δ, ppm): δ 7.76-7.70 (d, 2H), 7.64-7.61 (d, 4H), 7.56 (s, 2H), 7.43-7.41 (m, 5H), 7.39-7.35 (d, 2H), 7.27-7.22 (d, 1H), 7.08-7.05 (d, 1H), 6.66-6.54 (m, 4H), 5.35-5.31 (m, 4H), 5.24-5.17 (m, 2H), 5.14-5.09 (m, 4H), 4.97-4.90 (m, 5H), 4.86-4.73 (m, 3H), 4.67-4.57 (m, 4H), 4.53-4.34 (m, 9H), 4.10-4.04 (m, 10H), 4.01-3.95 (t, 2H), 3.88-3.86 (m, 7H), 3.82 (m, 3H), 2.16-2.14 (m, 19H), 2.09-2.05 (m, 46H), 2.03-1.97 (m, 18H), 1.58 (s, 6H), 1.26-1.21 (t, 4H). ^{13}C NMR (75.4 MHz, $CDCl_3$, δ, ppm): δ 170.56, 170.35, 170.28, 169.91, 161.43, 157.23, 136.63, 136.16, 129.13, 128.99, 127.61, 126.14, 117.58, 116.73, 101.12, 99.97, 72.74, 71.59, 71.49, 70.98, 70.68, 69.1, 66.61, 60.78, 53.8, 50.38, 31.74, 30.07, 29.24, 28.64, 20.91, 20.72, 20.49, 14.4.

BODIPY **3b** was prepared from BODIPY **2b** following the recipe described above to yield a green solid (65 mg, 55% yield). ^{1}H NMR (300 MHz, $CDCl_3$, δ, ppm): δ 7.81-7.75 (d, 2H), 7.62-7.60 (d, 4H), 7.44 (d, 4H), 7.41 (s, 2H), 7.39-7.34 (d, 2H), 7.25-7.20 (d, 2H), 7.05-7.03 (d, 1H), 6.63-6.55 (m, 2H), 5.36-5.34 (m, 2H), 5.21-5.07 (m, 4H), 5.00-4.86 (m, 6H), 4.69-4.66 (d, 2H), 4.57-4.46 (m, 8H), 4.14-4.04 (m, 10H), 3.90-3.78 (m, 6H), 3.68-3.6 (d, 2H), 2.65-2.63 (d, 4H), 2.16-2.14 (m, 16H), 2.10-2.05 (m, 23H), 2.02-1.97 (m, 10H), 1.90 (s, 4H), 1.72 (m, 2H), 1.60-1.54 (m, 6H), 1.48 (s, 6H), 1.25-1.20 (m, 4H), 1.18-1.15 (q, 6H). ^{13}C NMR (75.4 MHz, $CDCl_3$, δ, ppm): δ 170.49, 170.20, 169.89, 169.18, 161.41, 157.27, 149.83, 139.02, 137.24, 136.52, 135.69, 133.90, 133.62, 128.87, 128.35, 127.32, 120.0, 117.51, 106.09, 100.99, 99.78, 99.52, 72.61, 71.38, 70.94, 70.54, 69.03, 66.58, 61.72, 60.73, 53.70, 50.34, 29.98, 29.55, 28.63, 28.07, 23.13, 14.07, 11.14.

BODIPY **3c** was prepared from BODIPY **3b** following the recipe described above to yield a green solid (52 mg, 47% yield). ^{1}H NMR (300 MHz, $CDCl_3$, δ, ppm): δ 8.15-8.10 (s, 2H), 7.76 (s, 1H), 7.71 (s, 1H),

7.66-7.64 (d, 4H), 7.46-7.38 (m, 8H), 7.03-7.0 (d, 1H), 6.63-6.56 (d, 2H), 5.35 (m, 2H), 5.21-5.07 (m, 4H), 4.96-4.87 (m, 6H), 4.68 (d, 2H), 4.57-4.46 (m, 8H), 4.12-4.10 (m, 9H), 3.94-3.90 (m, 6H), 3.69-3.62 (m, 2H), 2.17-2.16 (m, 16H), 2.10-2.05 (m, 24H), 2.03-1.97 (m, 10H), 1.92 (s, 2H), 1.75 (m, 6H), 1.57 (s, 6H), 1.25-1.19 (m, 2H). ^{13}C NMR (75.4 MHz, $CDCl_3$, δ, ppm): δ 171.21, 170.93, 170.47, 169.88, 162.47, 157.67, 148.49, 141.86, 139.96, 137.42, 133.59, 130.11, 129.61, 128.38, 118.73, 116.8, 110.47, 106.96, 101.67, 100.14, 73.32, 71.25, 70.11, 69.67, 61.28, 54.46, 50.93, 32.34, 30.27, 29.83, 28.77, 23.69, 21.3, 21.2, 14.09.

LaB-*X* (X = H, Et, Br). The final compounds LaB-H, LaB-Et, and LaB-Br were obtained by the de-protonation of lactose acetate derivatives following the recipe as in our reported literature.[3] A representative procedure is described for the compound LaB-H.

BODIPY **3a** (100 mg) and sodium methoxide (20 mg) were dissolved in methanol (20 mL), which was stirred overnight at room temperature. The reaction mixture was neutralized by adding amber lite-resin H^+ (2 g) and filtered to separate the neutralized amberlite. After evaporating the solvent, the resulting crude product was re-crystallized using methanol/ether, filter, and washing by ether to yield the clean compound LaB-H (59 mg, 82% yield). ^{1}H NMR (400 MHz, $(CD_3)_2SO$, δ, ppm): δ 8.16 (s, 1H), 7.97 (s, 1H), 7.61-7.56 (m, 8H), 7.47-7.38 (m, 6H), 7.13 (d, 1H), 6.98 (s, 2H), 6.74-6.71 (t, 2H), 5.23-5.18 (d, 2H), 5.13 (t, 2H), 4.87-4.84 (m, 4H), 4.72-4.68 (m, 7H), 4.56 (s, 4H), 4.40 (s, 2H), 4.36-4.34 (d, 2H), 4.31-4.29 (d, 2H), 4.21 (s, 3H), 4.13 (s, 2H), 4.03 (s, 4H), 3.8 (s, 3H), 3.62 (s, 5H), 3.5 (m, 8H), 3.03 (m, 3H), 1.91 (s, 3H), 1.79 (s, 2H), 1.67 (s, 2H), 1.55 (s, 8H), 1.43 (s, 3H). ^{13}C NMR (100 MHz, $(CD_3)_2SO$, δ, ppm): δ 173.06, 161.34, 156.9, 151.66, 143.74, 141.92, 136.88, 136.43, 133.69, 129.38, 127.37, 124.06, 118.37, 115.38, 104.04, 101.95, 100.43, 80.85, 75.62, 75.06, 73.44, 73.23, 70.56, 68.20, 61.77, 60.45, 49.24, 29.69, 28.04, 22.79, 22.35, 14.01. HRMS (ESI): calculated for $C_{73}H_{93}BN_8O_{24}F_2Na$: 1537.6262; found: 1537.6257.

LaB-Et was prepared from BODIPY **3b** following the recipe described above to yield a green solid (57 mg, 75% yield). ^{1}H NMR (400 MHz, $(CD_3)_2SO$, δ, ppm): δ 8.16 (s, 1H), 7.99 (s, 1H), 7.65-7.54 (m, 6H), 7.47-7.40 (m, 4H), 7.38-7.3 (d, 2H), 7.27-7.25 (d, 2H), 7.09 (d, 1H), 6.75-6.71 (d, 2H), 5.21-5.16 (m, 2H), 5.12 (t, 2H), 4.86-4.81 (m, 4H), 4.72-4.67 (m, 8H), 4.54 (m, 4H), 4.40-4.35 (m, 4H), 4.29 (d, 1H), 4.20-4.13 (m, 2H), 4.04 (m, 3H), 4.01 (m, 3H), 3.81-3.78 (m, 4H), 3.62 (s, 4H), 3.51-3.45 (m, 7H), 3.05-3.02 (m, 4H), 2.63-2.61 (m, 4H), 1.93-1.90 (t, 4H), 1.80 (m, 2H), 1.67-1.66 (d, 2H), 1.56 (m, 2H), 1.46 (s, 6H), 1.24-1.22 (m, 2H), 1.12-1.09 (m, 6H). ^{13}C NMR (100 MHz, $(CD_3)_2SO$, δ, ppm): δ 170.09, 169.46, 161.55, 157.15, 149.43, 144.0, 139.38, 137.61, 137.17, 136.05, 133.84, 133.62, 129.72, 128.82, 127.45, 126.56, 124.59, 124.27, 119.7, 116.21, 107.14, 104.31, 102.27, 100.76, 81.22, 76.07, 75.44, 73.69, 70.98, 68.48, 62.17, 60.86, 49.19, 30.12, 29.68, 28.66, 28.01, 23.10, 22.71, 18.11, 14.48, 11.35. HRMS (ESI): calculated for $C_{77}H_{101}BN_8O_{24}F_2Na$: 1593.6888; found: 1593.6891.

LaB-Br was prepared from BODIPY **3c** following the recipe described above to yield a green solid (63 mg, 70% yield). ^{1}H NMR (400 MHz, $(CD_3)_2SO$, δ, ppm): δ 8.10-8.04 (s, 3H), 7.93 (s, 1H), 7.64-7.62 (d, 4H), 7.48-7.46 (d, 2H), 7.43 (d, 4H), 7.41 (d, 2H), 7.20-7.17 (d, 1H), 6.76-6.75 (d, 2H), 5.01-5.0 (m, 4H), 4.8-4.77 (m, 5H), 4.67-4.64 (m, 7H), 4.49 (m, 4H), 4.4 (d, 2H), 4.34 (m, 2H), 4.14-4.12 (d, 4H), 4.04-4.01 (d, 4H), 3.79-3.76 (d, 3H), 3.63 (s, 3H), 3.54-3.44 (m, 8H), 1.79 (m, 2H), 1.66 (d, 2H), 1.53 (s, 8H), 1.43

(m, 2H), 1.09 (m, 2H). ^{13}C NMR (100 MHz, $(CD_3)_2SO$, δ, ppm): δ 169.95, 169.66, 162.18, 156.95, 147.47, 143.57, 141.54, 139.32, 136.37, 132.91, 130.26, 129.69, 127.75, 124.67, 124.22, 117.78, 114.99, 110.03, 104.18, 99.2, 75.74, 75.41, 73.8, 71.24, 71.02, 68.25, 62.15, 60.63, 49.71, 31.2, 30.04, 29.44, 28.52, 22.99, 22.71, 21.06, 13.55. HRMS (ESI): calculated for $C_{73}H_{91}BN_8O_{24}F_2Br_2Na$: 1693.4472; found: 1693.4476.

S2. Determination of $^1O_2$ quantum yield of LaB-*X*

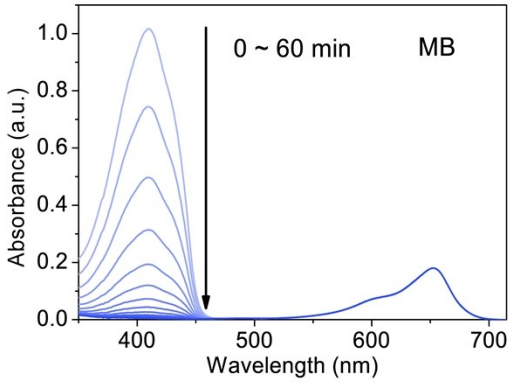

Figure S2. Time-dependent absorption spectra of air-saturated methanol solution of DPBF in the presence of methylene blue (MB) under red LED light irradiation (627 nm, 3 mW cm^{-2}).

S3. Theoretical characterization of the complete molecular structure

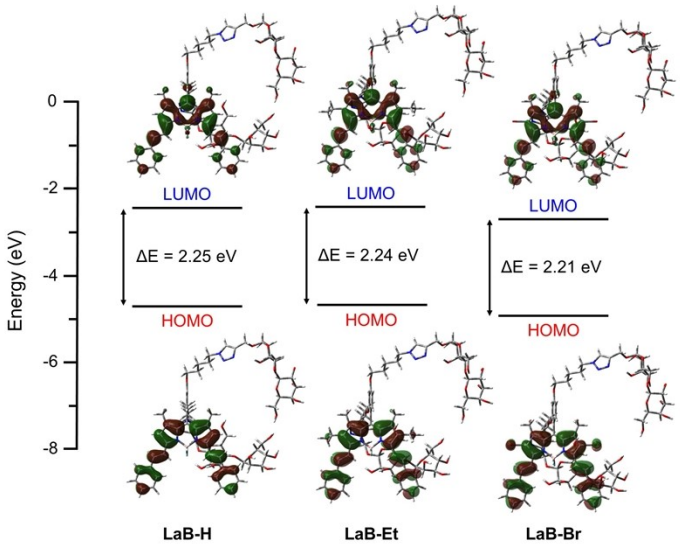

Figure S3. Energy level diagram and frontier molecular orbitals of the complete structure of LaB-*X*. The DFT calculations were performed under water solvent at the B3LYP/6-31G(d) level of theory.

S4. Morphological and spectroscopic characterization of LaB-*X* NPs

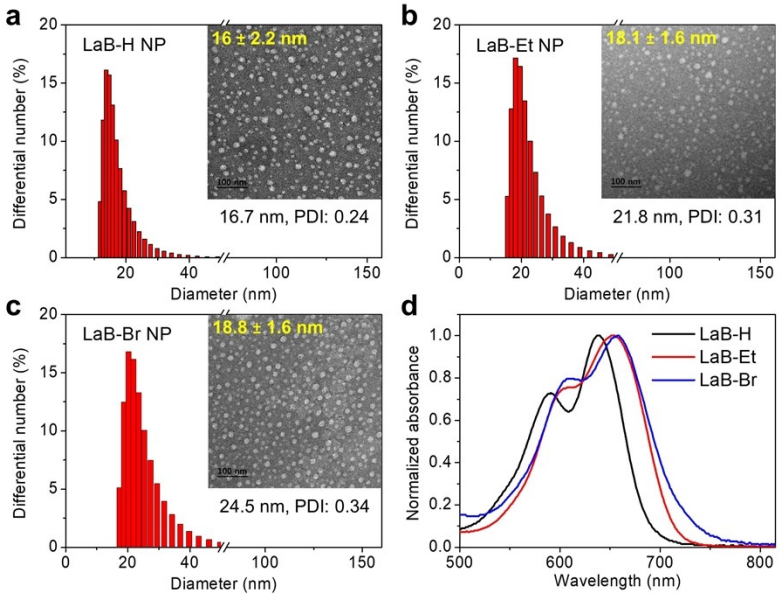

Figure S4. Histogram of hydrodynamic diameter (d_H) for (a) LaB-H-, (b) LaB-Et-, and (c) LaB-Br NPs prepared via dialysis and measured by DLS, with inset displaying a TEM image of the NP. Scale bar = 100 nm. (d) The normalized absorption spectra of LaB-*X* NP reported in panels a–c.

S5. Optimization of cell proliferation assay conditions

For cell proliferation assays, we preceded pre-experimentation to find optimal conditions for light irradiation dose and time. We chose Huh-7 cell as a test sample among three HCC cell lines, 1 and 5 μM as Lab-Br NP concentration for cell treatment, and 680 nm LED as a light source.

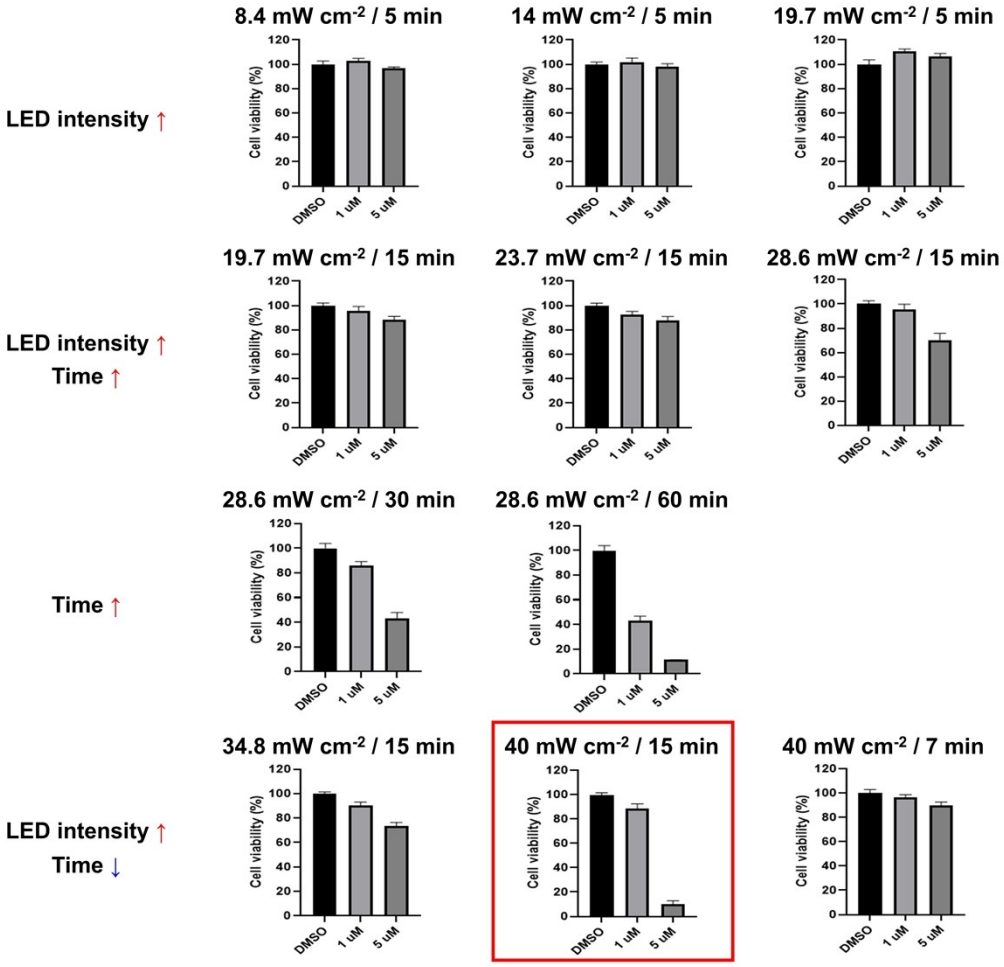

Figure S5. Viability of LaB-Br NP-treated Huh-7 cell depending on light irradiation dose and time.

Initially, we set the light irradiation time and dose to be 5 min and 8.4–19.7 mW cm^{-2}. Under these conditions, the cell viability barely changed for all conditions. Next, we increased both time and dose to 15 min and 19.7–28.6 mW cm^{-2}. A photocytotoxic effect was observed at the highest dose of 28.6 mW cm^{-2}, however, it was considered to be insufficient as the cell viability after 5 μM LaB-Br NP treatment was as

high as 70%. Next, we attempted two different ways: one is to further increase the time to 30 and 60 min while maintaining the dose at 28.6 mW cm^{-2} and the other is to further increase the dose to 34.8 and 40.0 mW cm^{-2} while maintaining the time as 15 min. A strong photocytotoxic effect was observed in the 28.6 mW cm^{-2}-60 min and 40.0 mW cm^{-2}-15 min conditions. Of the two conditions, we selected the 40.0 mW cm^{-2}-15 min condition as the final experimental condition, as long-term light exposure can cause thermal damage to cancer cells.

S6. Morphological change of cells by LaB-Br NP

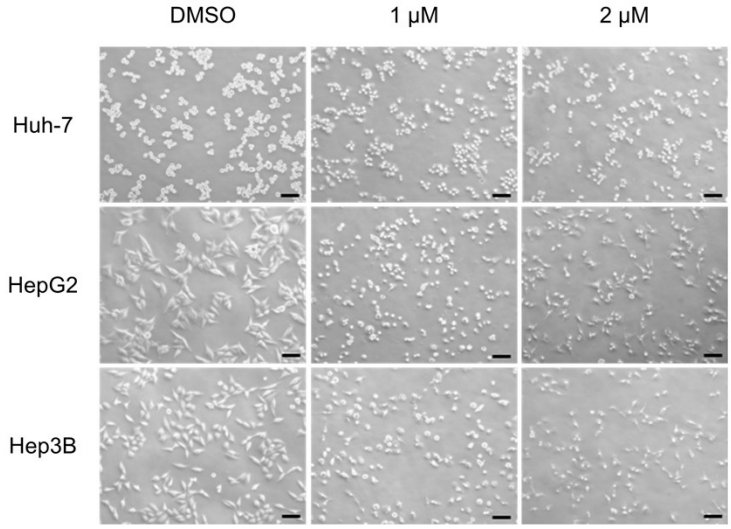

Figure S6. Morphology of HCC cells treated with LaB-Br (1 and 2 μM) and light irradiation (680 nm, 40 mW cm^{-2}, 15 min). After 12 h from treatment, the cells were imaged using a bright field microscope. Scale bar = 100 μm.

S7. Intracellular ROS generation by LaB-Br NP

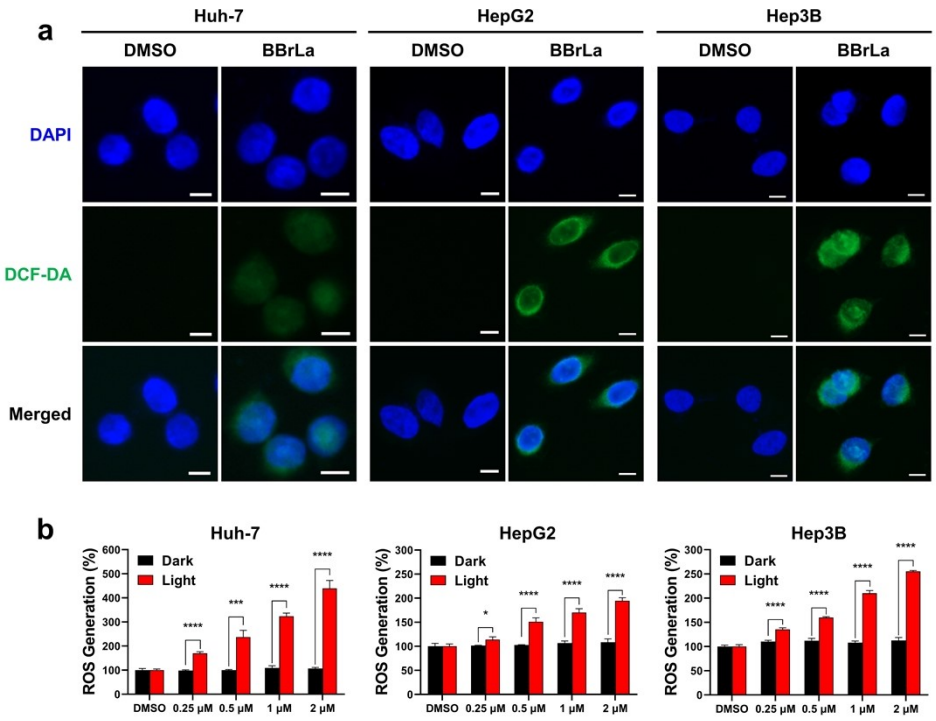

Figure S7. (a) Fluorescence images of DAPI- and DCFDA-costained HCC cells treated with LaB-Br (2 μM, 1 h) and light irradiation (680 nm, 40 mW cm^{-2}, 15 min). Scale bar = 10 μm. (b) Histograms illustrating ROS generation yield assessed after treatment of HCC cells with LaB-Br at different concentrations (0.25, 0.5, 1, and 2 μM) and with/without light irradiation (680 nm, 40 mW cm^{-2}, 15 min). Data are presented as mean ± standard deviation (n = 4). Statistical significance based on the Student's t-tests was considered as $^{**}p < 0.01$, $^{***}p < 0.001$, and $^{****}p < 0.0001$.

S8. NMR and MS spectra of LaB-*X* compounds

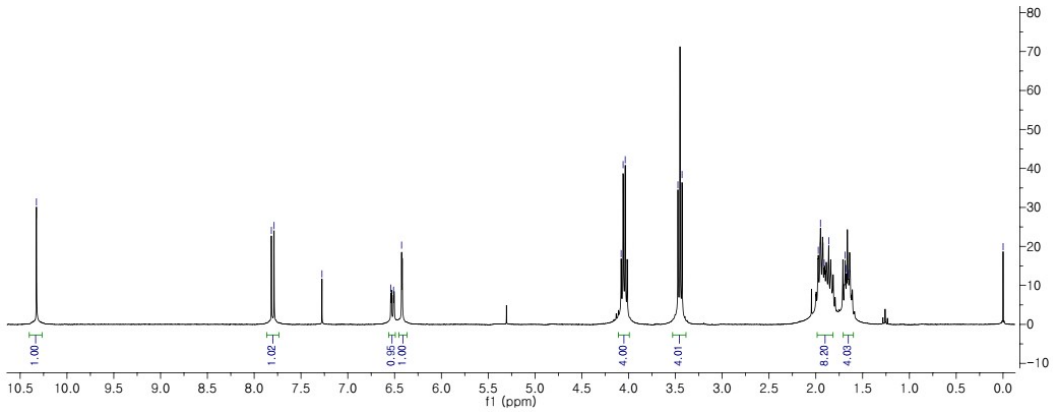

Figure S8. ^{1}H NMR spectrum of compound **2Br** in $CDCl_3$ at 300 MHz.

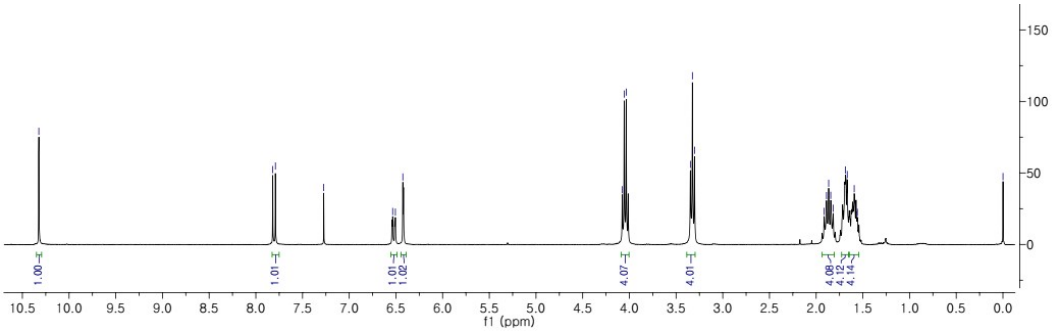

Figure S9. ^{1}H NMR spectrum of compound **2N$_3$** in $CDCl_3$ at 300 MHz.

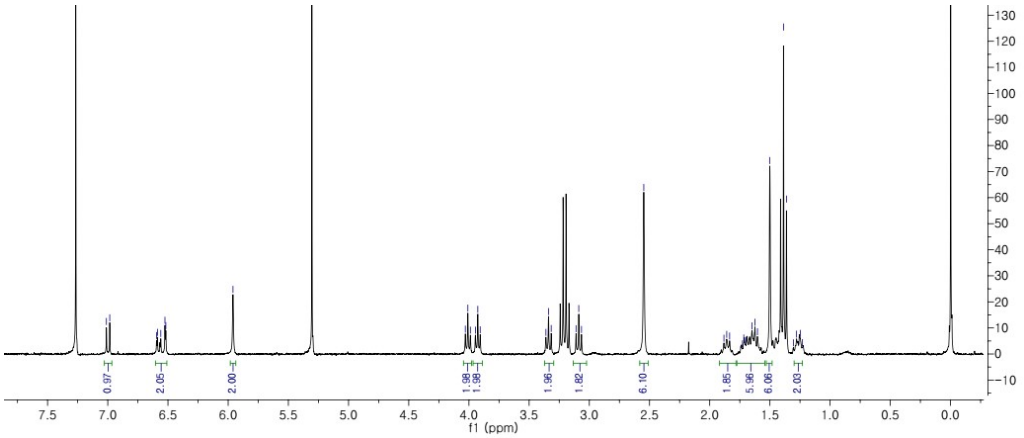

Figure S10. ^{1}H NMR spectrum of BODIPY **1a** in $CDCl_3$ at 300 MHz.

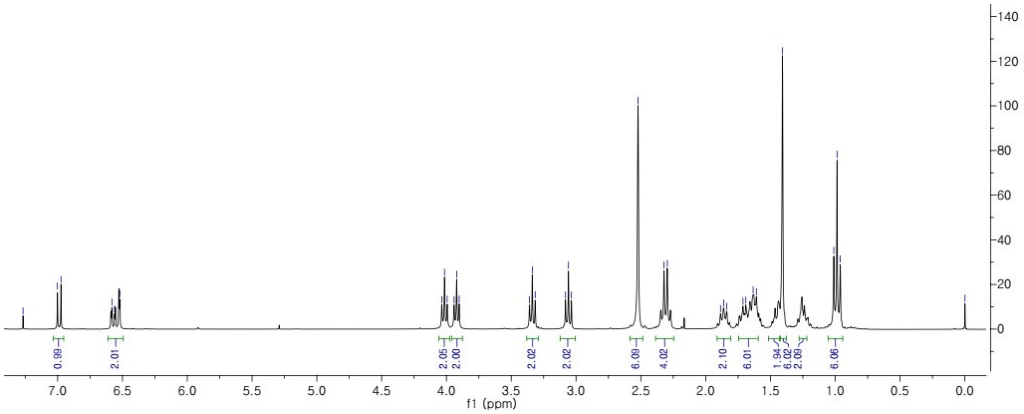

Figure S11. ^{1}H NMR spectrum of BODIPY **1b** in $CDCl_3$ at 300 MHz.

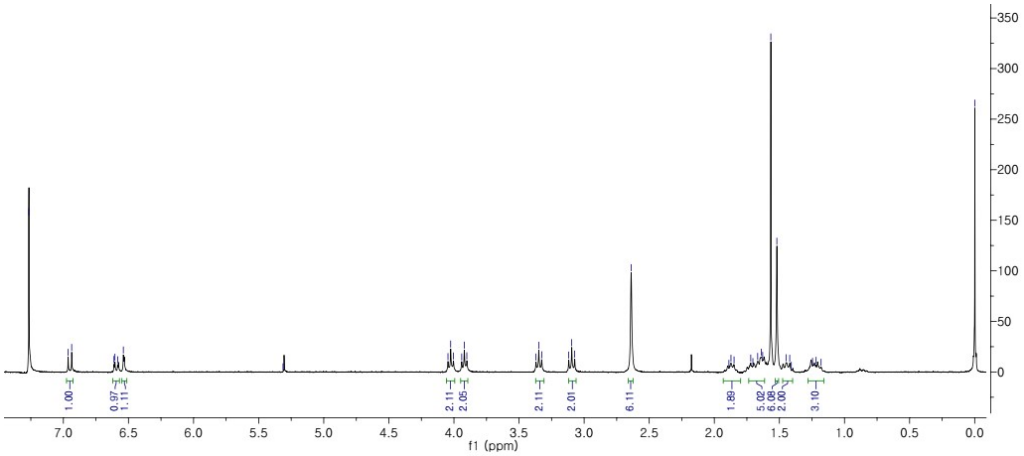

Figure S12. ^{1}H NMR spectrum of BODIPY **1c** in $CDCl_3$ at 300 MHz.

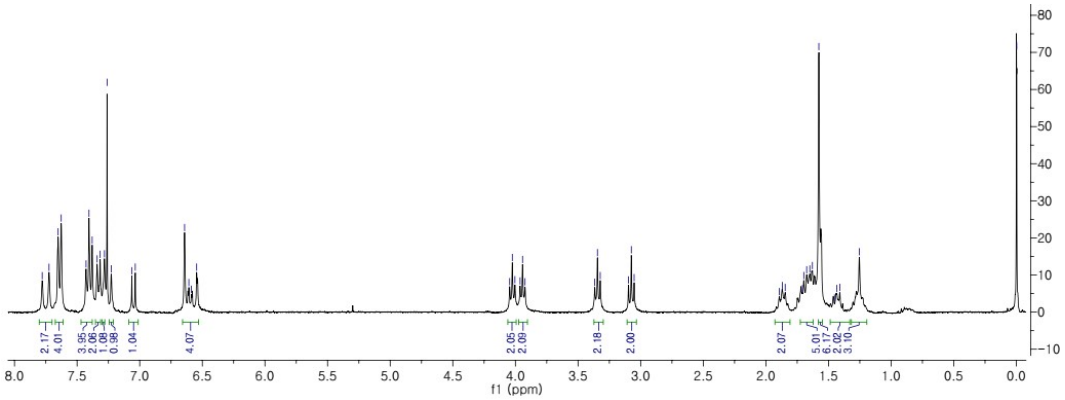

Figure S13. ^{1}H NMR spectrum of BODIPY **2a** in $CDCl_3$ at 300 MHz.

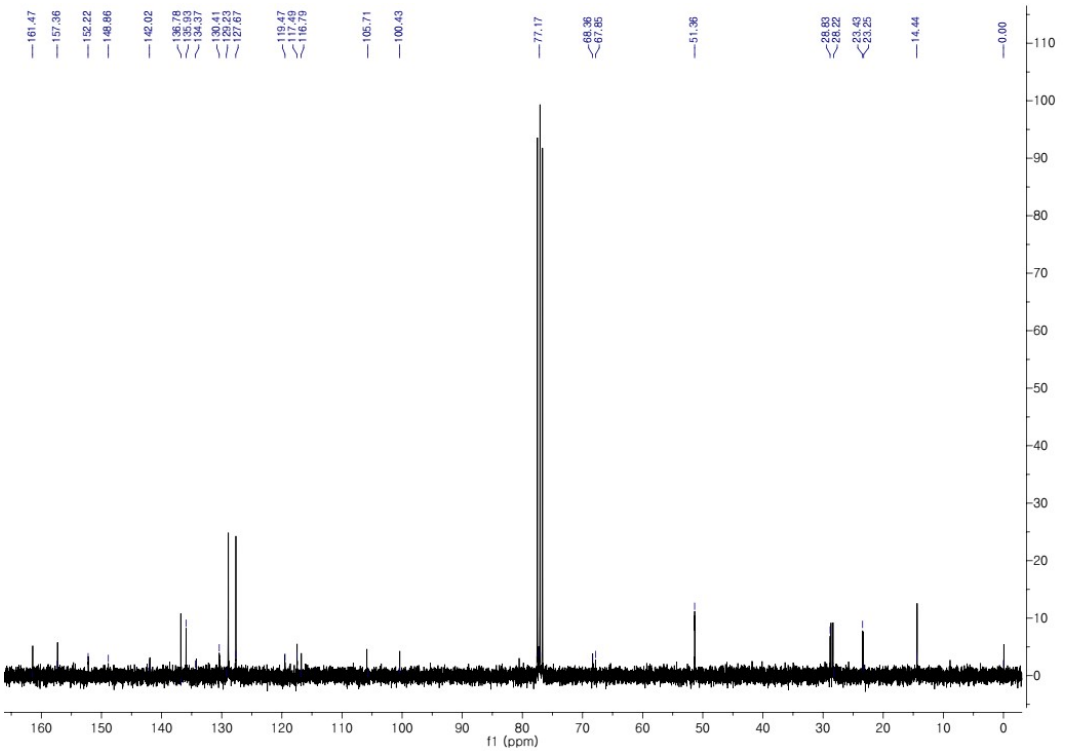

Figure S14. ^{13}C NMR spectrum of BODIPY **2a** in $CDCl_3$ at 75.4 MHz.

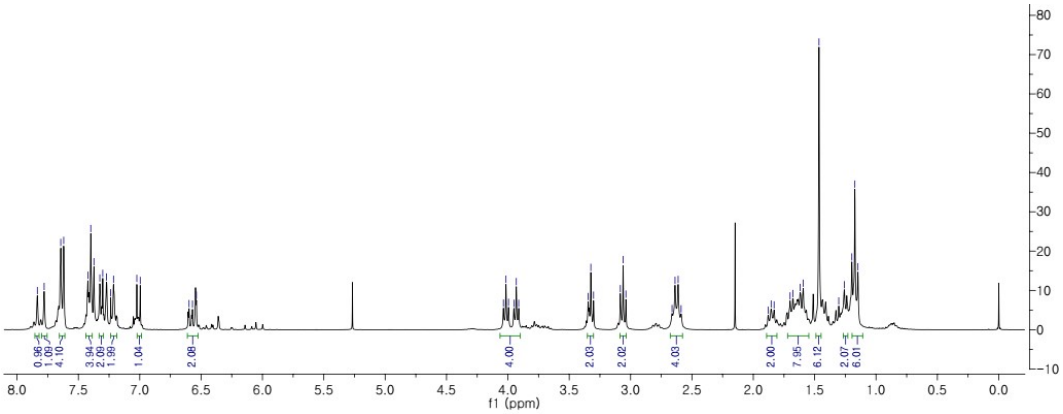

Figure S15. ^{1}H NMR spectrum of BODIPY **2b** in $CDCl_3$ at 300 MHz.

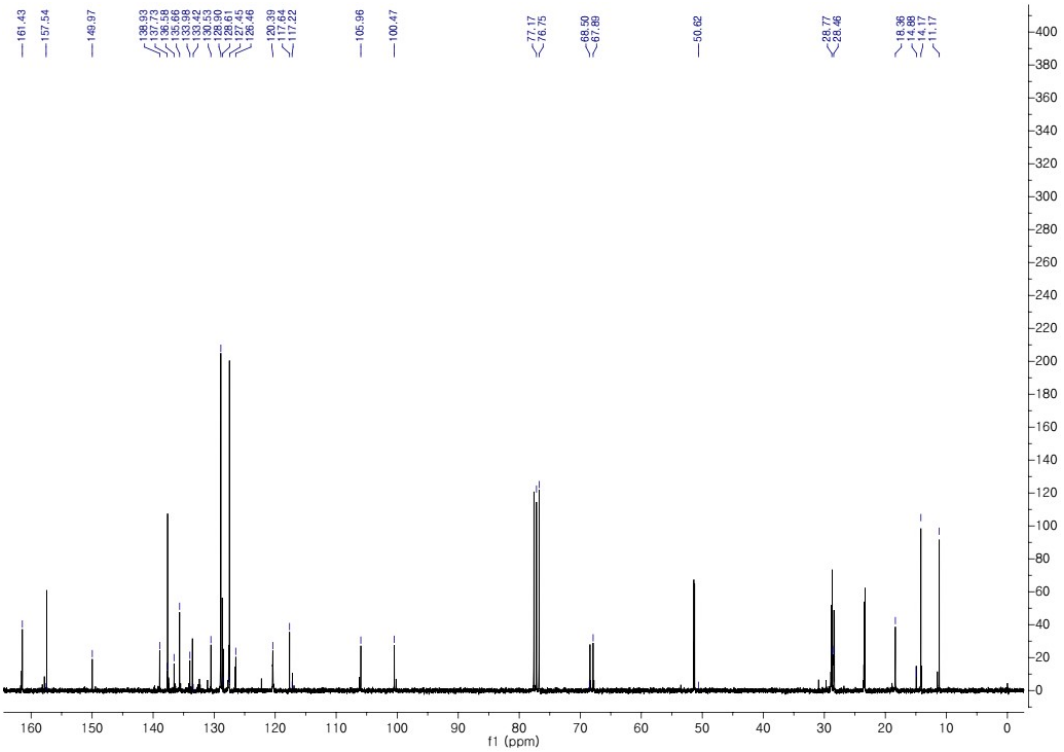

Figure S16. ^{13}C NMR spectrum of BODIPY **2b** in $CDCl_3$ at 75.4 MHz.

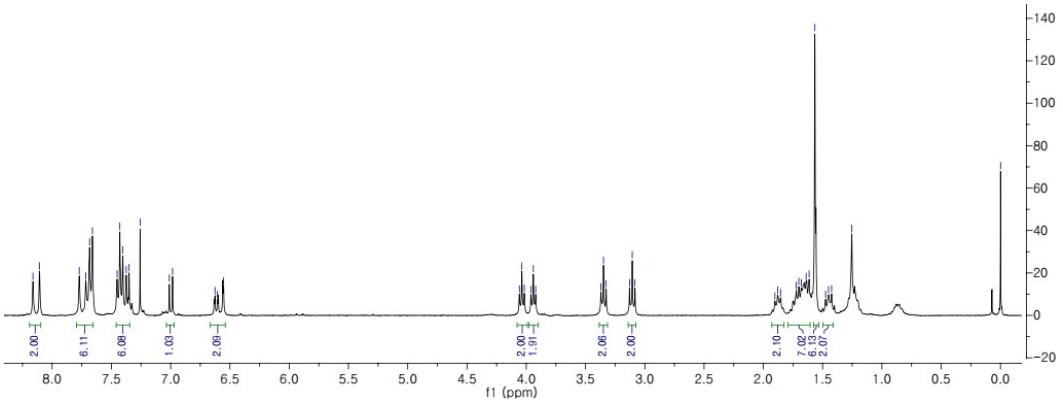

Figure S17. ^{1}H NMR spectrum of BODIPY **2c** in $CDCl_3$ at 300 MHz.

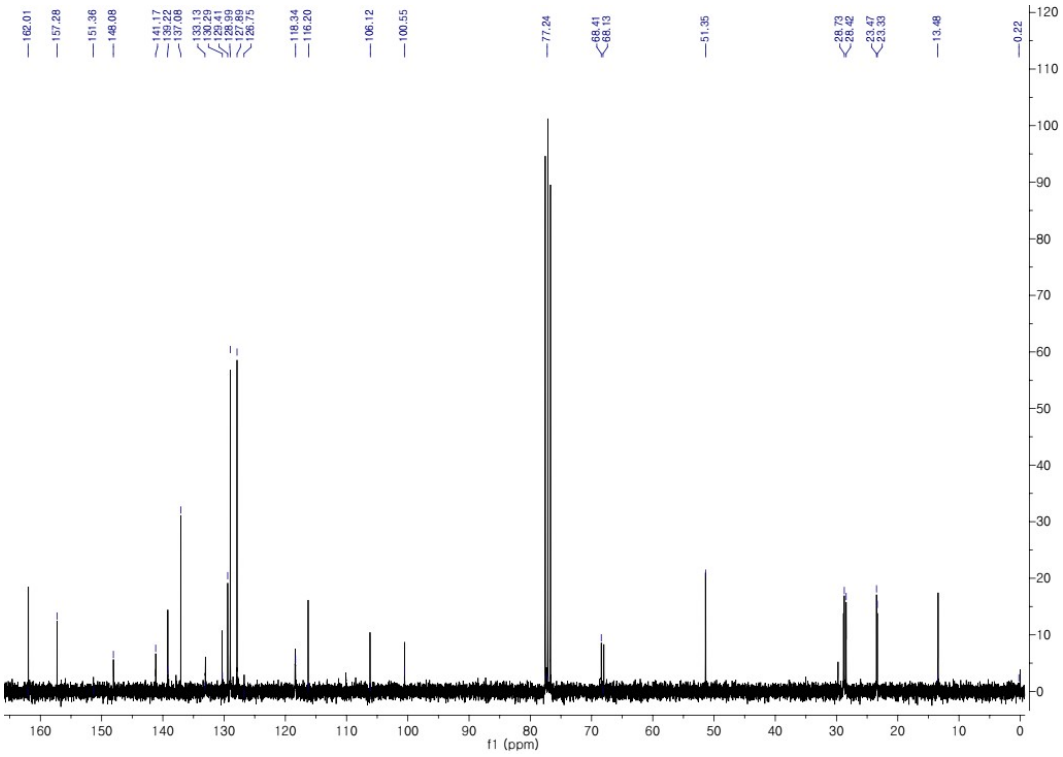

Figure S18. ^{13}C NMR spectrum of BODIPY **2c** in $CDCl_3$ at 75.4 MHz.

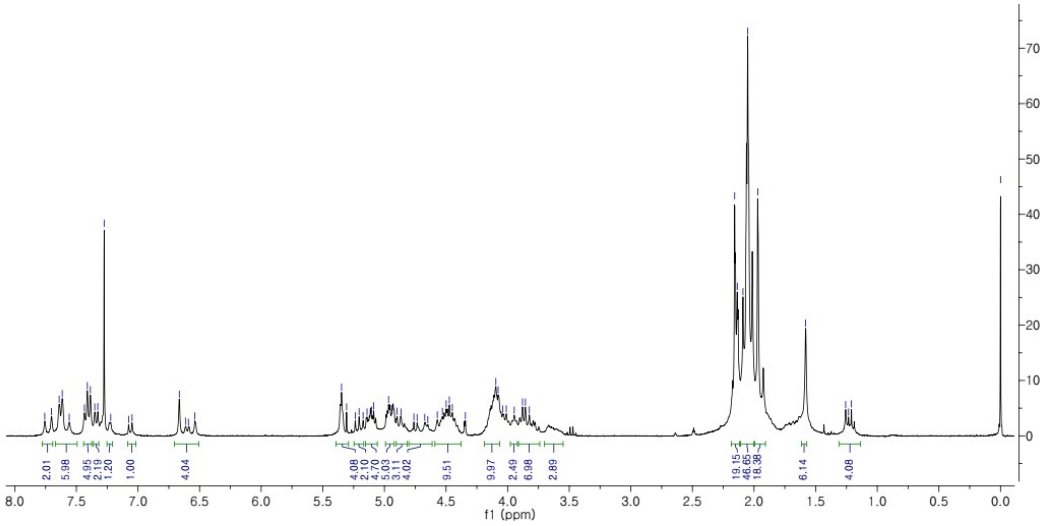

Figure S19. ^{1}H NMR spectrum of BODIPY **3a** in $CDCl_3$ at 300 MHz.

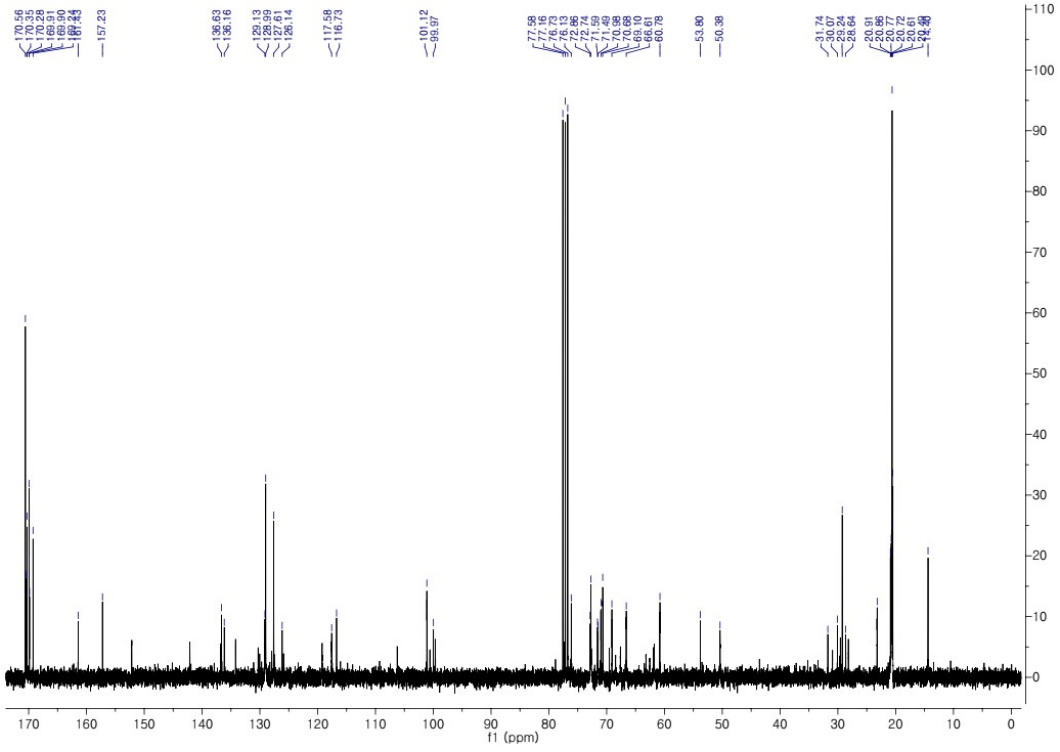

Figure S20. ^{13}C NMR spectrum of BODIPY **3a** in $CDCl_3$ at 75.4 MHz.

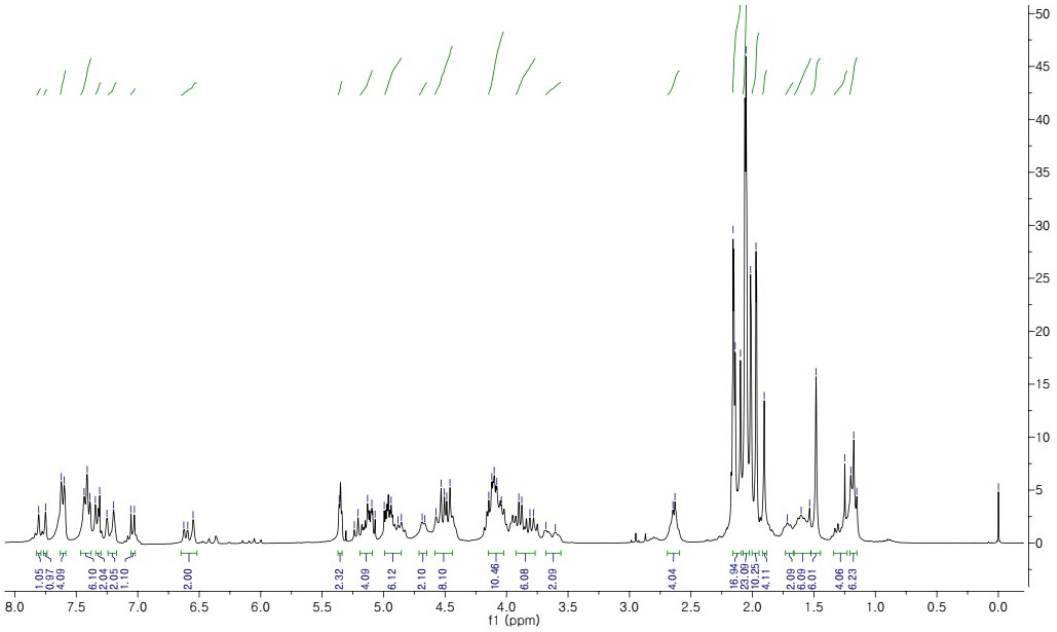

Figure S21. ^{1}H NMR spectrum of BODIPY **3b** in $CDCl_3$ at 300 MHz.

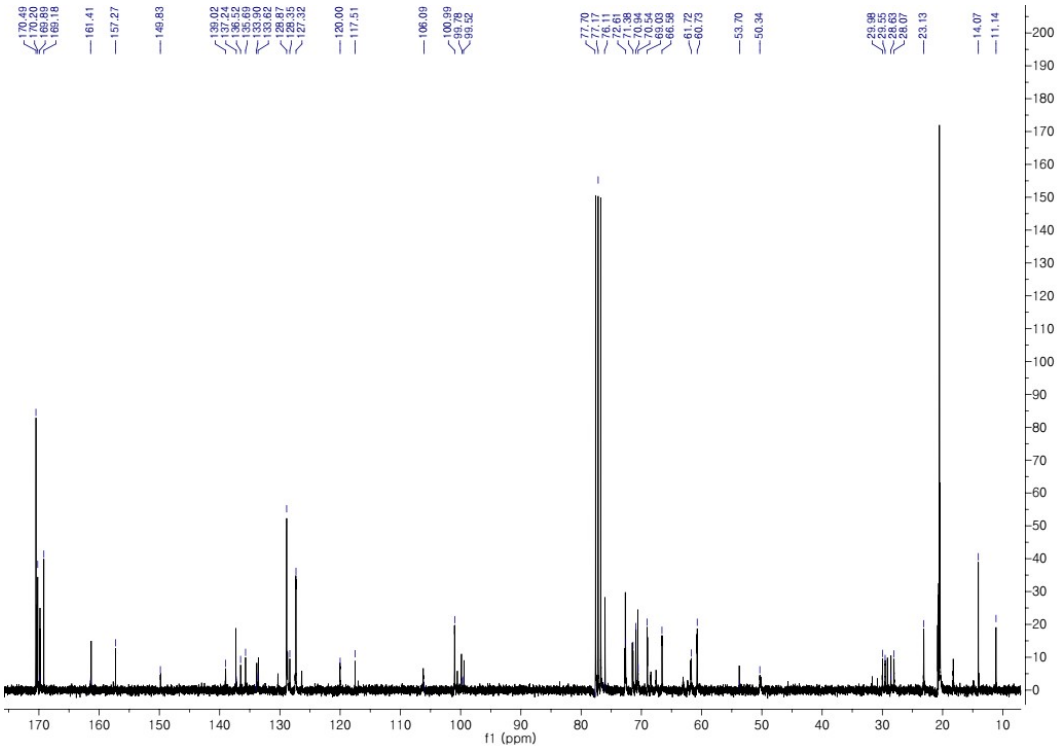

Figure S22. ^{13}C NMR spectrum of BODIPY **3b** in $CDCl_3$ at 75.4 MHz.

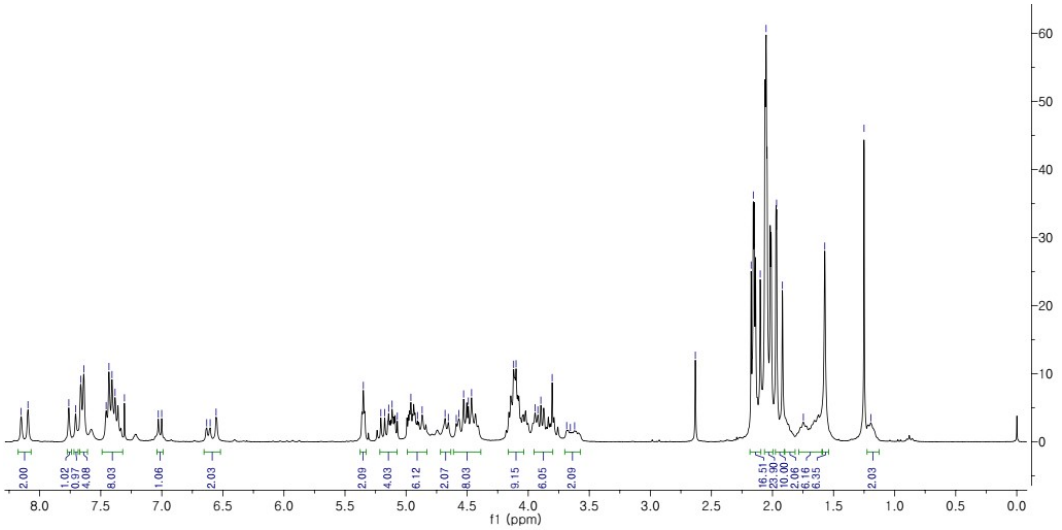

Figure S23. ^{1}H NMR spectrum of BODIPY **3c** in $CDCl_3$ at 300 MHz.

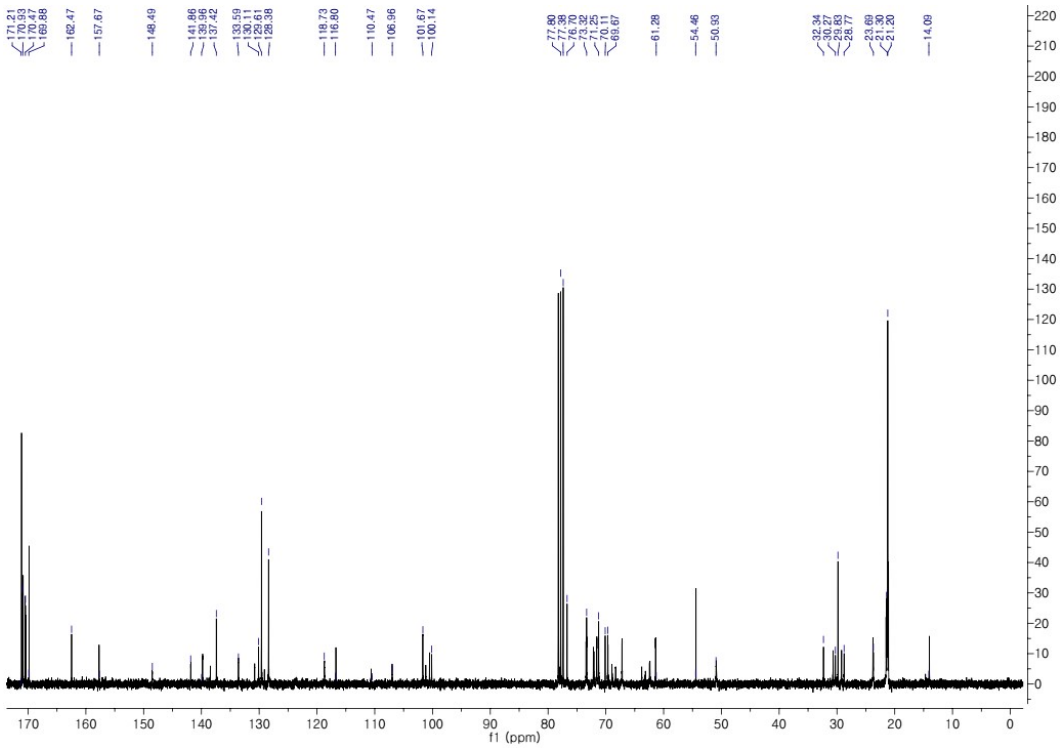

Figure S24. ^{13}C NMR spectrum of BODIPY **3c** in $CDCl_3$ at 75.4 MHz.

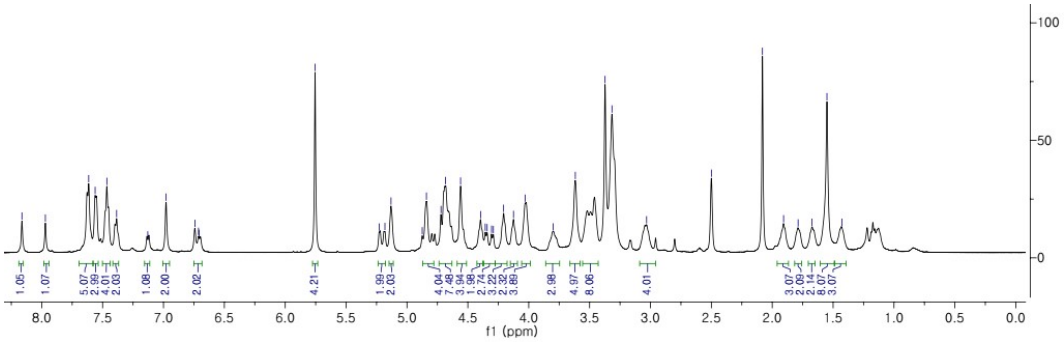

Figure S25. [1]H NMR spectrum of LaB-H in DMSO-d6 at 400 MHz.

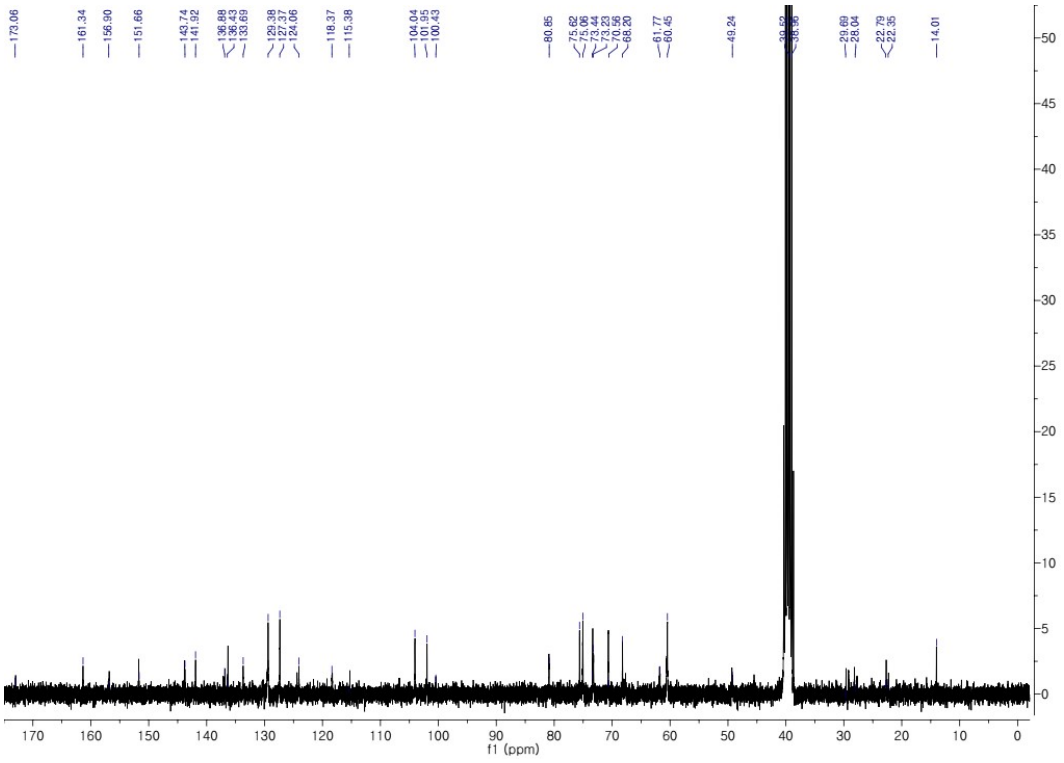

Figure S26. [13]C NMR spectrum of LaB-H in DMSO-d6 at 100 MHz.

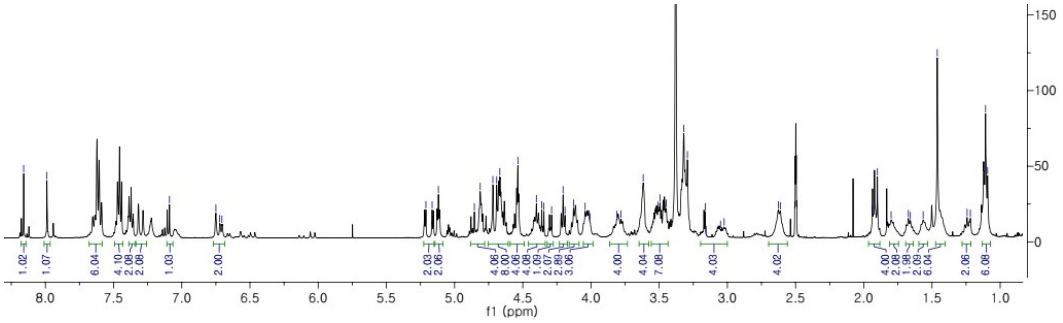

Figure S27. [1]H NMR spectrum of LaB-Et in DMSO-d6 at 400 MHz.

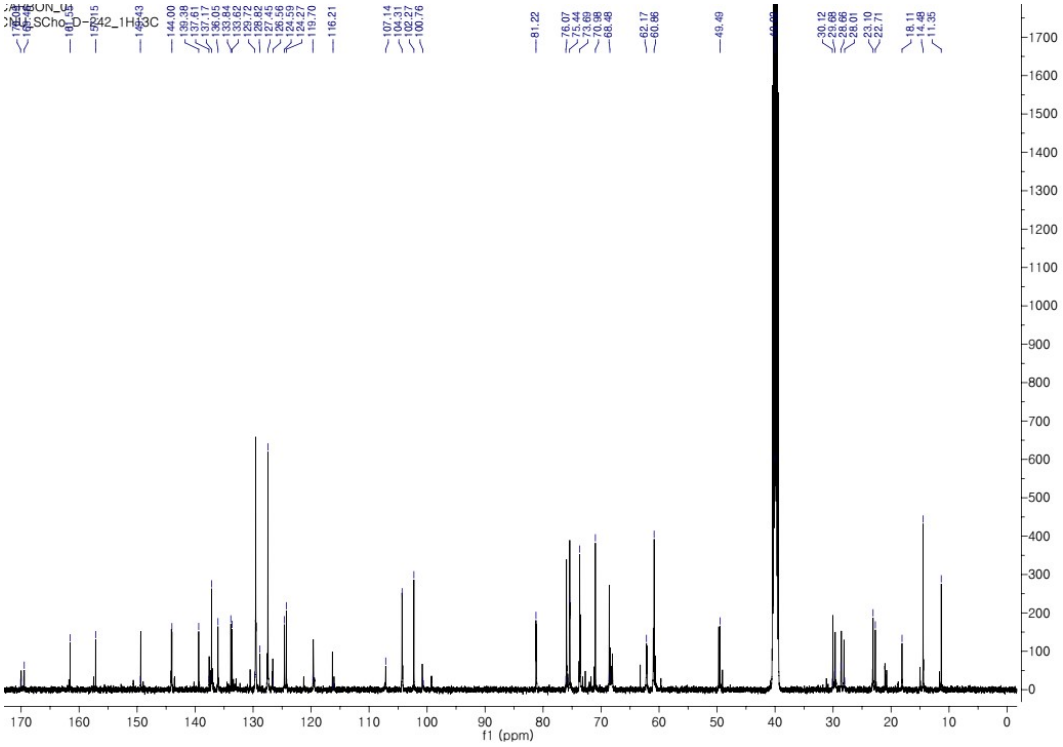

Figure S28. [13]C NMR spectrum of LaB-Et in DMSO-d6 at 100 MHz.

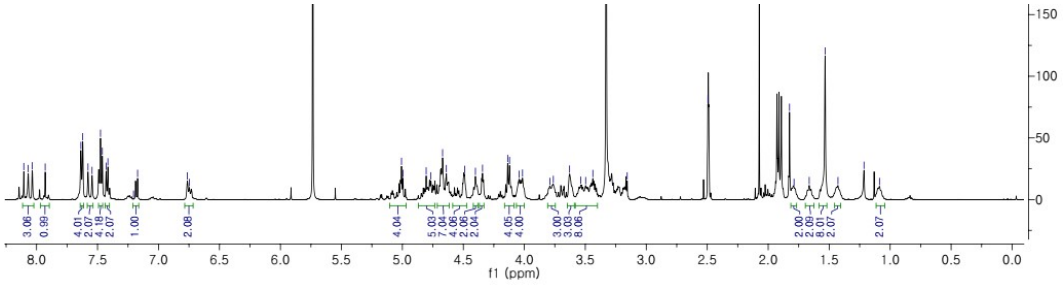

Figure S29. [1]H NMR spectrum of LaB-Br in DMSO-d6 at 400 MHz.

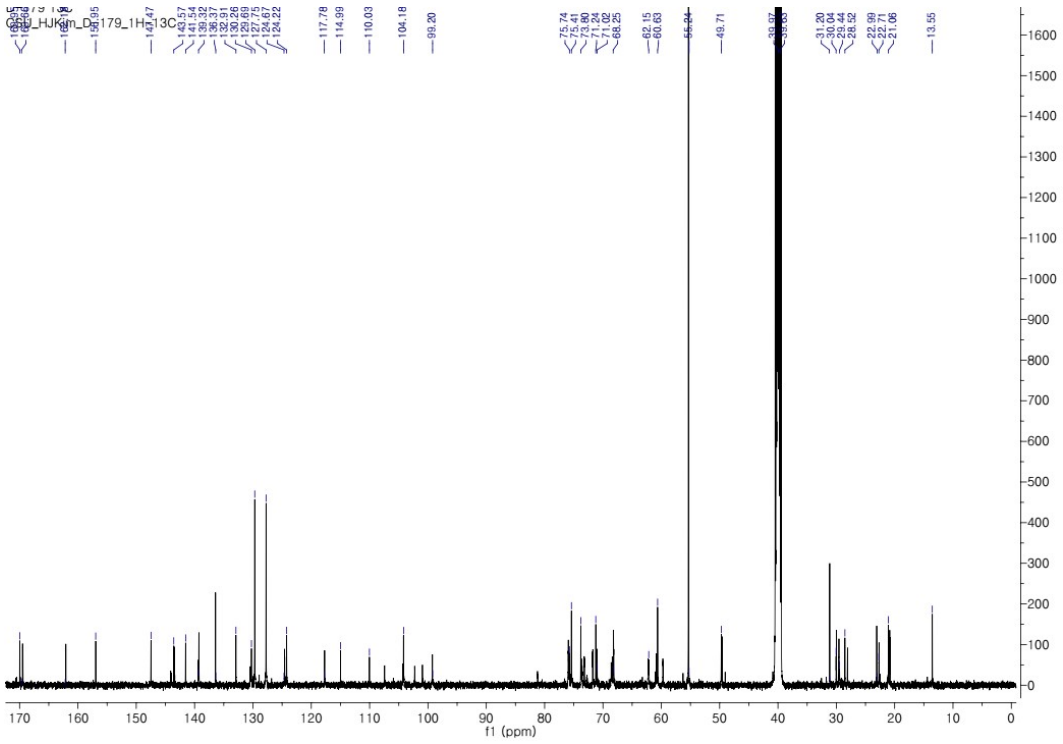

Figure S30. [13]C NMR spectrum of LaB-Br in DMSO-d6 at 100 MHz.

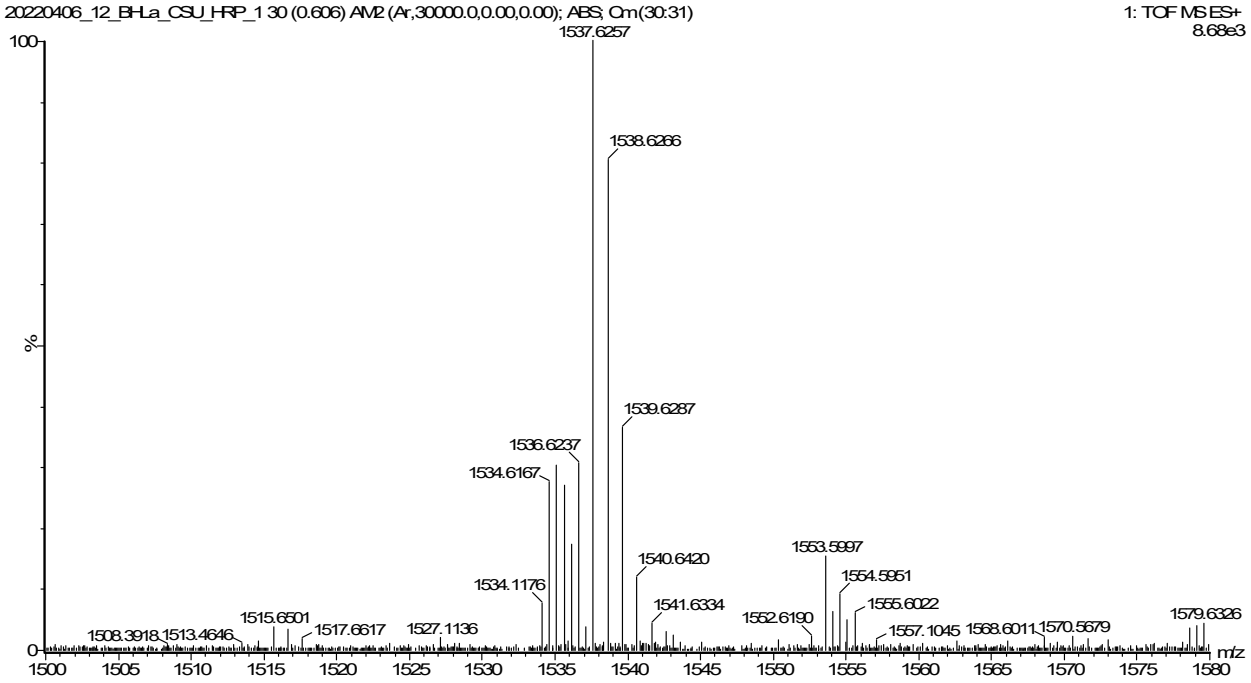

Figure S31. HRMS spectrum of BODIPY LaB-H.

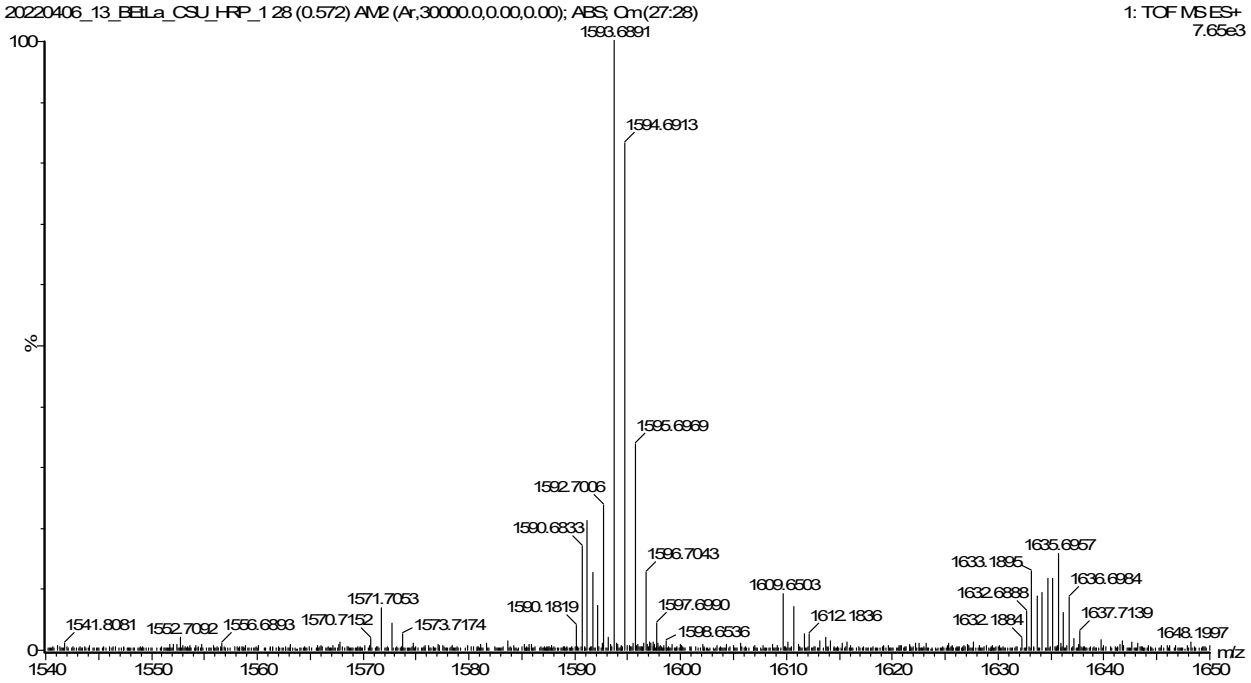

Figure S32. HRMS spectrum of BODIPY LaB-Et.

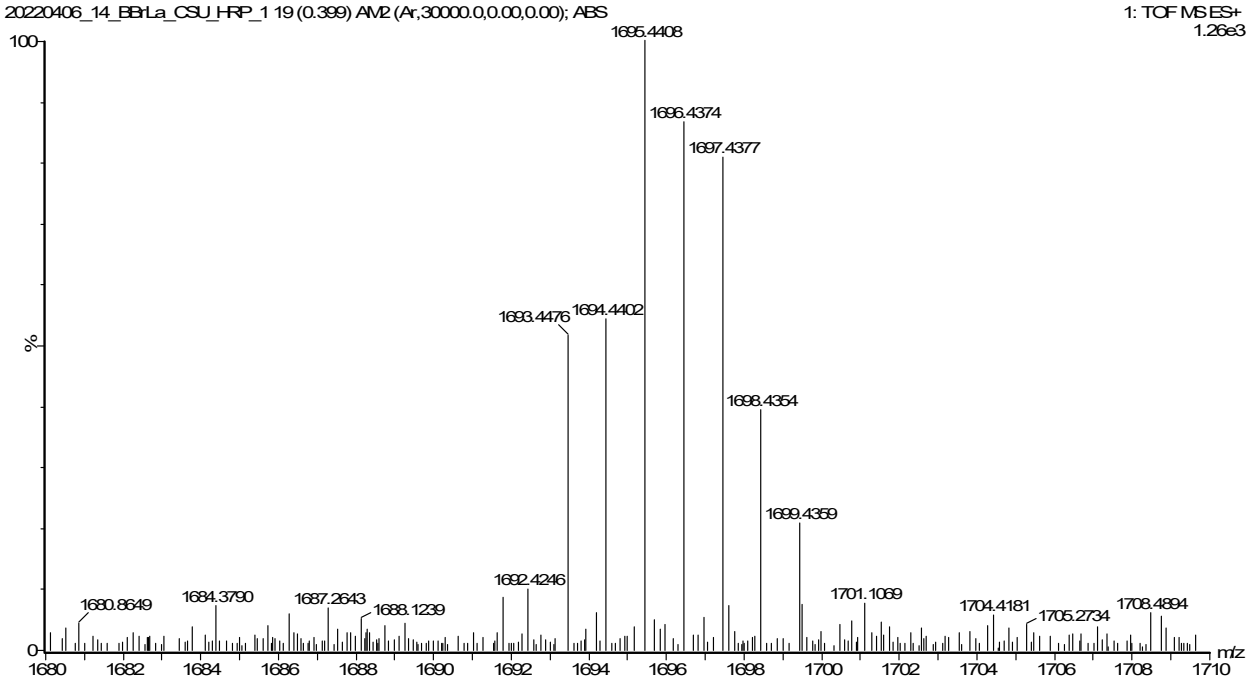

Figure S33. HRMS spectrum of BODIPY LaB-Br.

S9. References

1. Bui, H. T.; Mai, D. K.; Kim, B.; Choi, K.-H.; Park, B. J.; Kim, H.-J.; Cho, S., Effect of Substituents on the Photophysical Properties and Bioimaging Application of BODIPY Derivatives with Triphenylamine Substituents. *The Journal of Physical Chemistry B* **2019,** *123* (26), 5601-5607.
2. Kang, H.; Si, Y.; Liu, Y.; Zhang, X.; Zhang, W.; Zhao, Y.; Yang, B.; Liu, Y.; Liu, Z., Photophysical/Chemistry Properties of Distyryl-BODIPY Derivatives: An Experimental and Density Functional Theoretical Study. *The Journal of Physical Chemistry A* **2018,** *122* (25), 5574-5579.
3. Khuong Mai, D.; Kang, B.; Pegarro Vales, T.; Badon, I. W.; Cho, S.; Lee, J.; Kim, E.; Kim, H.-J., Synthesis and Photophysical Properties of Tumor-Targeted Water-Soluble BODIPY Photosensitizers for Photodynamic Therapy. *Molecules* **2020,** *25* (15), 3340.