Facile Synthesis of Near-Infrared Bodipy by Donor Engineering for In Vivo Tumor Targeted Dual-Modal Imaging

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1. Synthesis of Chemicals 1-6 (Figure 1)

1.1 Synthesis of Chemical 1

Bodipy (36.8 mg, 0.1 mmol) and benzaldehyde (31.8 mg, 0.3 mmol) were dissolved in the solution containing 18 ml anhydrous acetonitrile and 2 ml piperidine. After overnight reflux, the solution was dried with rotavapor and then redissolved in 4 ml DMF. The solution was purified by preparative chromatography (Agilent, 1260 Infinity) equipped with a C18 reversed-phase LC column (Luna 10 μm C18, 100 Å, LC column 250 × 21.2 mm), water/ACN: 90/10 to 10/90, linear gradient for 20 min, and then 90% ACN for further 20 min, with a flow rate of 12 mL/min. Ultrapure water and HPLC grade ACN [Sigma, St. Louis, MO, USA] were used. Chemical 1 was collected in fractions 25-26 min and lyophilized.

1H NMR (500 MHz, d6-DMSO, 25°C, TMS): δ 8.13 (d, J = 8.0 Hz, 2H), 7.65-7.53 (m, 10H), 7.48 (t, J = 7.5 Hz, 4H), 7.40 (t, J = 7.3 Hz, 2H), 7.03 (s, 2H), 1.42 (s, 6H); 13C NMR (125 MHz, d6-DMSO, 25°C, TMS): δ 167.38, 152.82, 142.40, 139.01, 138.62, 137.82, 136.51, 132.83, 132.06, 129.99, 129.69, 129.40, 127.75, 119.22, 118.52, 44.25, 22.71, 22.10, 14.87. HRMS (ESI) calc’d for [M] = [C34H27BF2N2O2]: 544.2134, calc’d for [M-H] = [C34H26BF2N2O2]: 543.2061, found [M-H]: 543.2049.

1.2 Synthesis of Chemical 2

Bodipy (36.8 mg, 0.1 mmol) and 4-formylbenzoic acid (45 mg, 0.3 mmol) were dissolved in the solution containing 18 ml anhydrous acetonitrile and 2 ml piperidine. After overnight reflux, the solution was dried with rotavapor and then redissolved in 4 ml DMF. The solution was purified by preparative chromatography (Agilent, 1260 Infinity) equipped with a C18 reversed-phase LC column (Luna 10 μm C18, 100 Å, LC column 250 × 21.2 mm), water/ACN: 90/10 to 10/90, linear gradient for 20 min, and then 90% ACN for further 30 min, with a flow rate of 12 mL/min. Ultrapure water and HPLC grade ACN [Sigma, St. Louis, MO, USA] were used. Chemical 2 was collected in fractions 20.5-22 min and lyophilized.

1H NMR (500 MHz, d6-DMSO, 25°C, TMS): δ 13.10 (s, 3H), 8.14 (d, J = 8.0 Hz, 2H), 8.03 (d, J = 8.2 Hz, 4H), 7.74 (d, J = 8.2 Hz, 4H), 7.72-7.63 (m, 6H), 7.08 (s, 2H), 1.43 (s, 6H); 13C NMR (125 MHz, d6-DMSO, 25°C, TMS): δ 167.36, 152.82, 142.40, 139.01, 138.62, 137.82, 136.51, 132.83, 132.06, 129.99, 129.69, 129.40, 127.75, 119.22, 118.52, 44.25, 22.71, 22.10, 14.87. HRMS (ESI) calc’d for [M] = [C36H29BF2N2O6]: 632.1930, calc’d for [M-H] = [C36H28BF2N2O6]: 631.1857, found [M-H]: 631.1840.

1.3 Synthesis of Chemical 3

Bodipy (36.8 mg, 0.1 mmol) and p-anisaldehyde (40.8 mg, 0.3 mmol) were dissolved in the solution containing 18 ml anhydrous acetonitrile and 2 ml piperidine. After overnight reflux, the solution was dried with rotavapor and then redissolved in 4 ml DMF. The solution was purified by preparative chromatography (Agilent, 1260 Infinity) equipped with a C18 reversed-phase LC column (Luna 10 μm C18, 100 Å, LC column 250 × 21.2 mm), water/ACN: 90/10 to 10/90, linear gradient for 20 min, and then 90% ACN for further 30 min, with a flow rate of 12 mL/min. Ultrapure water and HPLC grade ACN [Sigma, St. Louis, MO, USA] were used. Chemical 3 was collected in fractions 27-29 min and lyophilized.

1H NMR (500 MHz, d6-DMSO, 25°C, TMS): δ 8.12 (d, J = 8.2 Hz, 2H), 7.61-
7.54 (m, 8H), 7.41 (d, \(J = 16.3\) Hz, 2H), 7.05 (d, \(J = 8.8\) Hz, 4H), 6.96 (s, 2H), 3.82 (s, 6H), 1.40 (s, 6H); \(^{13}\)C NMR (125 MHz, d6-DMSO, 25°C, TMS): \(\delta 167.39, 162.81, 160.94, 158.35, 158.10, 152.92, 141.80, 139.23, 137.43, 137.39, 132.53, 131.94, 130.53, 129.52, 129.40, 129.29, 118.98, 118.80, 116.59, 116.33, 115.21, 55.85, 36.28, 31.26, 22.70, 14.84.

HRMS (ESI) calc’d for [M] = [C\(_{36}\)H\(_{31}\)BF\(_2\)N\(_2\)O\(_4\)]: 604.2345, calc’d for [M-H] = [C\(_{36}\)H\(_{30}\)BF\(_2\)N\(_2\)O\(_4\)]: 603.2272, found [M-H]: 603.2262.

1.4 Synthesis of Chemical 4

Bodipy (36.8 mg, 0.1 mmol) and \(p\)-hydroxybenzaldehyde (36.6 mg, 0.3 mmol) were dissolved in the solution containing 18 ml anhydrous acetonitrile and 2 ml piperidine. After overnight reflux, the solution was dried with rotavapor and then redissolved in 4 ml DMF. The solution was purified by preparative chromatography (Agilent, 1260 Infinity) equipped with a C18 reversed-phase LC column (Luna 10 \(\mu\)m C18, 100 Å, LC column 250 \times 21.2 mm), water/ACN: 90/10 to 10/90, linear gradient for 20 min, and then 90% ACN for further 30 min, with a flow rate of 12 mL/min. Ultrapure water and HPLC grade ACN [Sigma, St. Louis, MO, USA] were used. Chemical 4 was collected in fractions 21-22 min and lyophilized. \(^1\)H NMR (500 MHz, d6-DMSO, 25°C, TMS): \(\delta 13.27\) (s, 1H), 10.00 (s, 2H), 8.11 (d, \(J = 8.2\) Hz, 2H), 7.59 (d, \(J = 8.2\) Hz, 2H), 7.51-7.47 (m, 6H), 7.35 (d, \(J = 16.3\) Hz, 2H), 6.93 (s, 2H), 6.87 (d, \(J = 8.5\) Hz, 4H), 1.39 (s, 6H); \(^{13}\)C NMR (125 MHz, d6-DMSO, 25°C, TMS): \(\delta 179.98, 167.38, 159.58, 158.48, 158.23, 153.85, 152.99, 141.51, 139.33, 137.79, 136.84, 132.39, 131.88, 130.48, 129.57, 127.76, 118.61, 116.60, 115.39, 106.63, 105.51, 102.48, 98.53, 50.52, 44.22, 30.85, 28.70, 26.06, 24.14, 22.69, 22.09, 14.81, 14.36. HRMS (ESI) calc’d for [M] = [C\(_{34}\)H\(_{27}\)BF\(_2\)N\(_2\)O\(_4\)]: 576.2032, calc’d for [M-H] = [C\(_{34}\)H\(_{26}\)BF\(_2\)N\(_2\)O\(_4\)]: 575.1959, found [M-H]: 575.1946.

1.5 Synthesis of Chemical 5

Bodipy (36.8 mg, 0.1 mmol) and 4-(N,N-diphenylamino)benzaldehyde (82 mg, 0.3 mmol) were dissolved in the solution containing 18 ml anhydrous acetonitrile and 2 ml piperidine. After overnight reflux, the solution was dried with rotavapor and then redissolved in 4 ml DMF. The solution was purified by preparative chromatography (Agilent, 1260 Infinity) equipped with a C18 reversed-phase LC column (Luna 10 \(\mu\)m C18, 100 Å, LC column 250 \times 21.2 mm), water/ACN: 80/20 to 0/100, linear gradient for 20 min, and then 100% ACN for further 30 min, with a flow rate of 12 mL/min. Ultrapure water and HPLC grade ACN [Sigma, St. Louis, MO, USA] were used. Chemical 5 was collected in fractions 39-42 min and lyophilized. \(^1\)H NMR (500 MHz, d6-DMSO, 25°C, TMS): \(\delta 13.27\) (s, 1H), 10.00 (s, 2H), 8.11 (d, \(J = 8.2\) Hz, 2H), 7.59 (d, \(J = 8.2\) Hz, 2H), 7.51-7.47 (m, 6H), 7.35 (d, \(J = 16.3\) Hz, 2H), 6.93 (s, 2H), 6.87 (d, \(J = 8.5\) Hz, 4H), 1.39 (s, 6H); \(^{13}\)C NMR (125 MHz, d6-DMSO, 25°C, TMS): \(\delta 179.98, 167.38, 159.58, 158.48, 158.23, 153.85, 152.99, 141.51, 139.33, 137.79, 136.84, 132.39, 131.88, 130.48, 129.57, 127.76, 118.61, 116.60, 115.39, 106.63, 105.51, 102.48, 98.53, 50.52, 44.22, 30.85, 28.70, 26.06, 24.14, 22.69, 22.09, 14.81, 14.36. HRMS (ESI) calc’d for [M] = [C\(_{58}\)H\(_{45}\)BF\(_2\)N\(_2\)O\(_2\)]: 878.3604, calc’d for [M-H] = [C\(_{58}\)H\(_{44}\)BF\(_2\)N\(_2\)O\(_2\)]: 877.3531, found [M-H]: 877.3513.

1.6 Synthesis of Chemical 6

Bodipy (36.8 mg, 0.1 mmol) and 4-dimethylaminobenzaldehyde (44.8 mg, 0.3 mmol) were dissolved in the solution containing 18 ml anhydrous acetonitrile and 2 ml piperidine. After
overnight reflux, the solution was dried with rotavapor and then redissolved in 4 ml DMF. The solution was purified by preparative chromatography (Agilent, 1260 Infinity) equipped with a C18 reversed-phase LC column (Luna 10 μm C18, 100 Å, LC column 250 × 21.2 mm), water/ACN: 90/10 to 10/90, linear gradient for 20 min, and then 90% ACN for further 30 min, with a flow rate of 12 mL/min. Ultrapure water and HPLC grade ACN [Sigma, St. Louis, MO, USA] were used. Chemical 6 was collected in fractions 23-25 min and lyophilized. 

\(^1\)H NMR (500 MHz, d6-DMSO, 25°C, TMS): \(\delta\) 8.10 (d, \(J = 7.8\) Hz, 2H), 7.58-7.55 (m, 2H), 7.33-7.27 (m, 2H), 6.89 (s, 2H), 6.81 (d, \(J = 8.0\) Hz, 4H), 3.01 (s, 12H), 1.38 (s, 6H); 

\(^13\)C NMR (125 MHz, d6-DMSO, 25°C, TMS): \(\delta\) 167.41, 158.81, 158.52, 152.84, 151.43, 140.75, 137.84, 131.75, 130.50, 130.40, 129.73, 129.55, 129.34, 129.28, 118.34, 112.81, 112.73, 44.24, 22.70, 14.79. HRMS (ESI) calc’d for [M] = [C\(_{38}\)H\(_{37}\)BF\(_2\)N\(_4\)O\(_2\)]: 630.2978, calc’d for [M+H]\(^+\) = [C\(_{38}\)H\(_{38}\)BF\(_2\)N\(_4\)O\(_2\)]\(^+\): 631.3056, found [M+H]\(^+\): 631.3052.

2. The normalized absorption and emission spectra of Chemicals 1-6 in DMSO.

![Figure S1. The normalized absorption and emission spectra of Chemical 1 in DMSO.](image1)

![Figure S2. The normalized absorption and emission spectra of Chemical 2 in DMSO.](image2)
Figure S3. The normalized absorption and emission spectra of Chemical 3 in DMSO.

Figure S4. The normalized absorption and emission spectra of Chemical 4 in DMSO.

Figure S5. The normalized absorption and emission spectra of Chemical 5 in DMSO.
Figure S6. The normalized absorption and emission spectra of Chemical 6 in DMSO.

3. The MALDI-TOF characterization of PEGylated 5.

Figure S7. The MALDI-TOF characterization of PEGylated 5. The arrow indicates the MW corresponding to the condensation reaction between the chemical 5 and the mean-MW-PEG2000 species.

4. The $^1$H NMR characterization of PEGylated 5.
5. The critical micelle concentration (CMC) value of PEGylated 5.
The CMC value of PEGylated 5 was estimated by the curves of the maximal emission wavelength of Pyrene in the presence of PEGylated 5 NPs at various concentrations (0.125 μM, 0.25 μM, 0.5 μM, 0.8 μM, 2 μM, 4 μM, 8 μM). The PEGylated 5 NPs solutions were prepared by diluting from 200 μM PEGylated 5 NPs solution. 20 μL Pyrene solution in acetone was added to 2 mL PEGylated 5 NPs solutions, then the mixtures were aged for 4 h. After 4 hours, the fluorescence spectra of Pyrene were measured (with the excitation wavelength of 330 nm, excitation slit width of 20 nm and emission slit width 2.5 nm) and analyzed to plot the curve for the estimation of the CMC value. The first spectral band at 373 nm ($I_1$) and the third spectral band at 383 nm ($I_3$) of Pyrene were recorded for plotting the CMC curve with concentration as abscissa and $I_1/I_3$ ratio as ordinate. To obtain the
CMC value, two trend lines were drawn and their intersection was defined as CMC.

Figure S9. PEGylated 5 exhibited a critical micelle concentration of 0.942 μM.

6. The biocompatibility test (MTS assay) of NIR NPs with A549 lung cancer cells.

Figure S10. The cytoviability of A549 cancer cells after incubation with the NIR NPs at different concentrations for 24 h and 48 h, respectively.

7. The biocompatibility test (MTS assay) of NIR NPs with Human umbilical vein endothelial cells (HUVEC) cells.
Figure S11. The cytoviability of HUVEC cells after incubation with the NIR NPs at different concentrations for 24 h.

8. The $^1$H NMR, $^{13}$C NMR and HRMS (ESI) characterizations of Chemicals 1-6.

Chemical 1:

\[ 
\begin{align*}
\text{HO} & \quad \text{O} \\
& \quad \text{N} \quad \text{B} \quad \text{N} \\
& \quad \text{F} \quad \text{F} \\
\end{align*}
\]

$^1$H NMR (500 MHz, d6-DMSO, 25°C, TMS): $\delta$ 8.13 (d, $J = 8.0$ Hz, 2H), 7.65-7.53 (m, 10H), 7.48 (t, $J = 7.5$ Hz, 4H), 7.40 (t, $J = 7.3$ Hz, 2H), 7.03 (s, 2H), 1.42 (s, 6H); $^{13}$C NMR (125 MHz, d6-DMSO, 25°C, TMS): $\delta$ 167.38, 152.82, 142.40, 139.01, 138.62, 137.82, 136.51, 132.83, 132.06, 130.61, 129.99, 129.69, 129.40, 127.75, 119.22, 118.52, 44.25, 22.71, 22.10, 14.87. HRMS (ESI) calc’d for [M]=[C$_{34}$H$_{27}$BF$_2$N$_2$O$_2$]: 544.2134, calc’d for [M-H]$^-$=[C$_{34}$H$_{26}$BF$_2$N$_2$O$_2$]: 543.2061, found [M-H]$^-$: 543.2049.
Chemical 2:

\[ \text{HO-COO} \]

\[ \text{HO} \]

\[ \text{O} \]

\[ \text{F} \]

\[ \text{F} \]

\[ \text{N} \]

\[ \text{N} \]

\[ \text{B} \]

\[ \text{N} \]

\[ \text{N} \]

\[ \text{C}_{34} \text{H}_{27} \text{B} \text{F}_2 \text{N}_2 \text{O}_2 \]

\[ 1^H \text{NMR (500 MHz, d}_6\text{-DMSO, 25°C, TMS): } \delta 13.10 (s, 3H), 8.14 (d, J = 8.0 Hz, 2H), 8.03 (d, J = 8.2 Hz, 4H), 7.74 (d, J = 8.2 Hz, 4H), 7.72-7.63 (m, 6H), 7.08 (s, 2H), 1.43 (s, 6H); \]

\[ ^{13}C \text{ NMR (125 MHz, d}_6\text{-DMSO, 25°C, TMS): } \delta 167.36, 167.33, 152.57, 142.76, 140.55, 139.32, 138.80, 136.77, 133.26, 132.12, 131.44, 130.61, 129.31, 127.77, 120.47, 119.69, 14.89. \]

Chemical 3:

1H NMR (500 MHz, d6-DMSO, 25°C, TMS): \( \delta \) 8.12 (d, \( J = 8.2 \) Hz, 2H), 7.61-7.54 (m, 8H), 7.41 (d, \( J = 16.3 \) Hz, 2H), 7.05 (d, \( J = 8.8 \) Hz, 4H), 6.96 (s, 2H), 3.82 (s, 6H), 1.40 (s, 6H); 13C NMR (125 MHz, d6-DMSO, 25°C, TMS): \( \delta \) 167.39, 162.81, 160.94, 158.35, 158.10, 152.92, 141.80, 139.23, 137.43, 137.39, 132.53, 131.94, 130.53, 129.52, 129.40, 129.29, 118.98, 118.80, 116.59, 116.33, 115.21, 55.85, 36.28, 31.26, 22.70, 14.84. HRMS (ESI) calc’d for [M]=[C36H30BF2N2O4]: 604.2345, calc’d for [M-H]: [C36H30BF2N2O4]-: 603.2272, found [M-H]: 603.2262.
Chemical 4:

\[
\text{HO} \quad \begin{array}{c}
\text{CO} \\
\text{N} \quad \text{N} \\
\text{F} \\
\text{B} \\
\text{F} \\
\text{N} \quad \text{N} \\
\text{CO} \\
\text{HO}
\end{array}
\]

\(^1\text{H} \text{ NMR} (500 \text{ MHz, d6-DMSO, 25}^\circ\text{C, TMS}): \delta 13.27 \text{ (s, 1H), 10.00 (s, 2H), 8.11 (d, } J = 8.2 \text{ Hz, 2H), 7.59 (d, } J = 8.2 \text{ Hz, 2H), 7.51-7.47 (m, 6H), 7.35 (d, } J = 16.3 \text{ Hz, 2H), 6.93 (s, 2H), 6.87 (d, } J = 8.5 \text{ Hz, 4H), 1.39 (s, 6H); } ^{13}\text{C NMR (125 MHz, d6-DMSO, 25}^\circ\text{C, TMS): } \delta 179.98, 167.38, 159.58, 158.48, 158.23, 153.85, 152.99, 141.51, 139.33, 137.79, 136.84, 132.39, 131.88, 130.48, 129.57, 127.76, 118.61, 116.60, 115.39, 106.63, 105.51, 102.48, 98.53, 50.52, 44.22, 30.85, 28.70, 26.06, 24.14, 22.69, 22.09, 14.81, 14.36. \text{ HRMS (ESI) calc'd for [M]=[C}_{34}\text{H}_{27}\text{BF}_2\text{N}_2\text{O}_4]: 576.2032, calc’d for [M-H]= [C}_{34}\text{H}_{26}\text{BF}_2\text{N}_2\text{O}_4]: 575.1959, found [M-H]: 575.1946.
Chemical 5:

\[ \text{HO\textsuperscript{\textbullet\textbullet}} \]

\[ \begin{array}{c}
\text{N} \\
\text{F} \\
\text{N} \\
\text{N} \\
\text{N} \\
\text{N} \\
\text{N} \\
\text{N} \\
\text{N} \\
\text{N} \\
\text{N} \\
\text{N} \\
\text{N} \\
\text{N} \\
\end{array} \]

\[ \text{C}_{34}\text{H}_{27}\text{B}\text{F}_{2}\text{N}_{2}\text{O}_{4} \cdot \text{ESI Scan (0.002, 0.011, 0.019, 0.027 ... min, 48 Scans) Frag=365.0} \]

\[ \text{575.1946} \]

\[ ([\text{C}_{34}\text{H}_{27}\text{B}\text{F}_{2}\text{N}_{2}\text{O}_{4}]\text{-H})^{-} \]

\[ \text{Counts vs. Mass-to-Charge (m/z)} \]

\[ \begin{array}{c}
\text{1H NMR (500 MHz, d6-DMSO, 25°C, TMS):} \\
\delta 8.11 \text{ (d, } J = 8.3 \text{ Hz, 2H), 7.95 (s, 1H), 7.60} \\
\text{ (s, 2H), 7.49 (d, } J = 7.9 \text{ Hz, 4H), 7.40-7.34 (m, 10H), 7.15-7.09 (m, 12H), 6.96 (d, } J = 5.6} \\
\text{Hz, 6H), 6.38 (s, 1H), 2.36, 2.33 (s, s, 6H);} \\
\text{13C NMR (125 MHz, d6-DMSO, 25°C, TMS):} \]
\end{array} \]

Not available due to the poor solubility in DMSO. HRMS (ESI) calc’d for [M]=[C\text{58}H\text{45}BF\text{2}N\text{4}O\text{2}]: 878.3604, calc’d for [M-H]:=\text{[C\text{58}H\text{44}BF\text{2}N\text{4}O\text{2}]: 877.3531, found [M-H]: 877.3513.}
Chemical 6:
\(^1\)H NMR (500 MHz, d6-DMSO, 25°C, TMS): \(\delta 8.10 \text{ (d, } J = 7.8 \text{ Hz, } 2\text{H}), 7.58-7.55 \text{ (m, } 2\text{H}), 7.48-7.43 \text{ (m, } 6\text{H}), 7.33-7.27 \text{ (m, } 2\text{H}), 6.89 \text{ (s, } 2\text{H}), 6.81 \text{ (d, } J = 8.0 \text{ Hz, } 4\text{H}), 3.01 \text{ (s, } 12\text{H}), 1.38 \text{ (s, } 6\text{H}); \(^{13}\)C NMR (125 MHz, d6-DMSO, 25°C, TMS): \(\delta 167.41, 158.81, 158.52, 152.84, 151.43, 140.75, 137.84, 131.75, 130.50, 130.40, 129.73, 129.55, 129.34, 129.28, 118.34, 112.81, 112.73, 44.24, 22.70, 14.79. \) HRMS (ESI) calc’d for [M]=[C\(_{38}\)H\(_{37}\)BF\(_2\)N\(_4\)O\(_2\)]: 630.2978, calc’d for [M+H]\(^+\)=[C\(_{38}\)H\(_{38}\)BF\(_2\)N\(_4\)O\(_2\)]: 631.3056, found [M+H]\(^+\): 631.3052.
Cpd 1: C38H37BF2N4O2+: FBF Spectrum (rt: 1.339-1.364 min) an-0904-1.d Subtract

631.3052
([C38H37BF2N4O2]+H)^+