

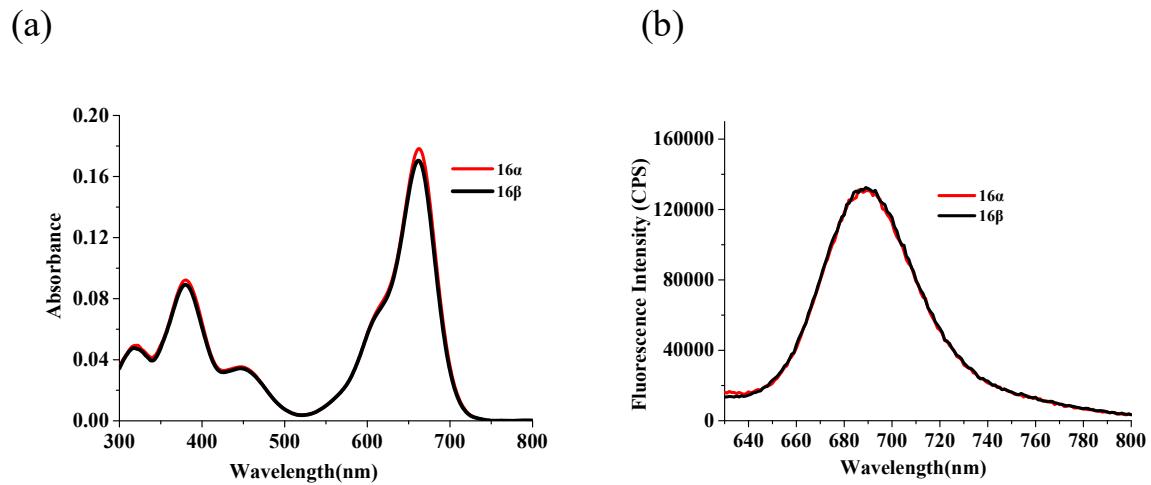
## Supplementary Materials

# Comparison of the In Vitro Photodynamic Activity of the C<sub>1α</sub> and C<sub>1β</sub> Anomers of a Glucosylated Boron Dipyrromethene

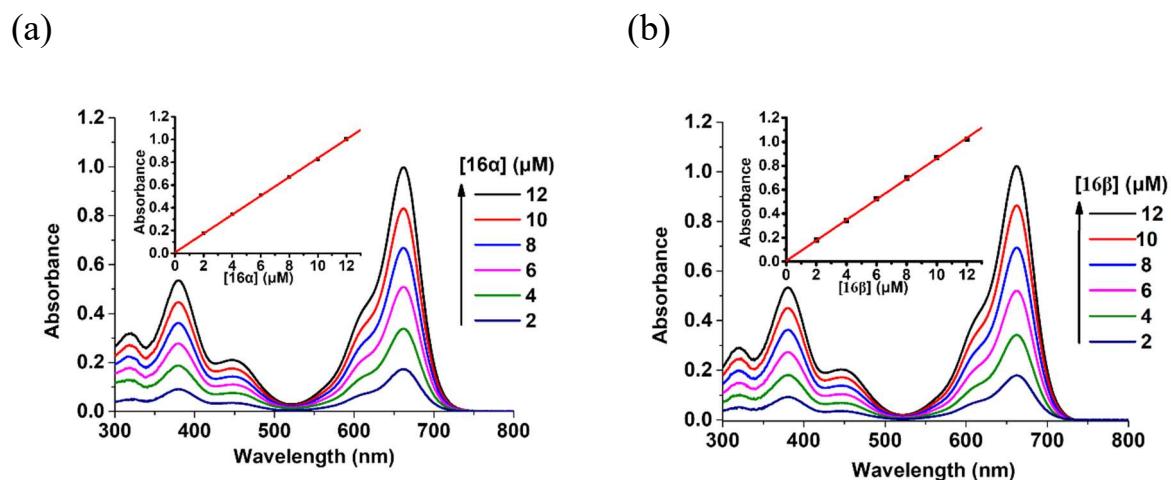
Junlong Xiong, Ka-Wing Yeung, Clarence T. T. Wong, Wing-Ping Fong and Dennis K. P. Ng

## Contents

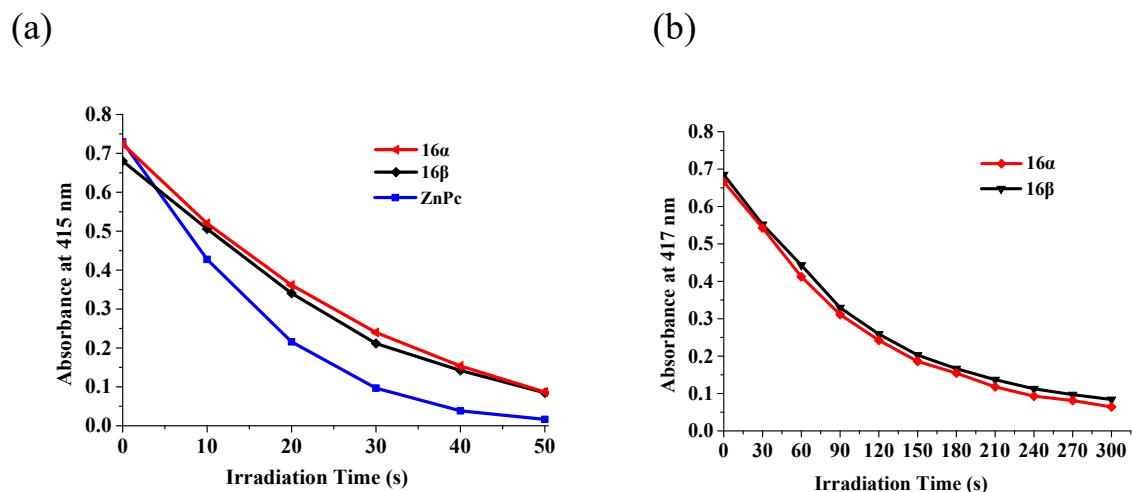
- Figure S1** (a) Electronic absorption and (b) fluorescence (excited at 610 nm) spectra of **16α** and **16β** (both at 2 μM) in DMF.
- Figure S2** UV-Vis spectra of (a) **16α** and (b) **16β** at different concentrations in DMF.
- Figure S3** Comparison of the rate of photodecay of DPBF (initial concentration = 30 μM) in (a) DMF and (b) PBS (pH = 7.4) with 0.1% Tween 80 (v/v) using **16α**, **16β**, and ZnPc (all at 2 μM) as the photosensitizers.
- Figure S4** (a) Electronic absorption and (b) fluorescence (excited at 610 nm) spectra of **16α** and **16β** (both at 2 μM) in PBS (pH = 7.4) with 0.1% Tween 80 (v/v).
- Figure S5** <sup>1</sup>H (top) and <sup>13</sup>C{<sup>1</sup>H} (bottom) NMR spectra of **3** in CDCl<sub>3</sub>.
- Figure S6** <sup>1</sup>H (top) and <sup>13</sup>C{<sup>1</sup>H} (bottom) NMR spectra of **4** in CDCl<sub>3</sub>.
- Figure S7** <sup>1</sup>H (top) and <sup>13</sup>C{<sup>1</sup>H} (bottom) NMR spectra of **6** in CDCl<sub>3</sub>.
- Figure S8** <sup>1</sup>H (top) and <sup>13</sup>C{<sup>1</sup>H} (bottom) NMR spectra of **9** in CDCl<sub>3</sub>.
- Figure S9** <sup>1</sup>H (top) and <sup>13</sup>C{<sup>1</sup>H} (bottom) NMR spectra of **10** in CDCl<sub>3</sub>.
- Figure S10** <sup>1</sup>H (top) and <sup>13</sup>C{<sup>1</sup>H} (bottom) NMR spectra of **11** in CDCl<sub>3</sub>.
- Figure S11** <sup>1</sup>H (top) and <sup>13</sup>C{<sup>1</sup>H} (bottom) NMR spectra of **14β** in CDCl<sub>3</sub>.
- Figure S12** <sup>1</sup>H (top) and <sup>13</sup>C{<sup>1</sup>H} (bottom) NMR spectra of **14α** in CDCl<sub>3</sub>.
- Figure S13** <sup>1</sup>H (top) and <sup>13</sup>C{<sup>1</sup>H} (bottom) NMR spectra of **15β** in CDCl<sub>3</sub>.
- Figure S14** <sup>1</sup>H (top) and <sup>13</sup>C{<sup>1</sup>H} (bottom) NMR spectra of **15α** in CDCl<sub>3</sub>.
- Figure S15** <sup>1</sup>H (top) and <sup>13</sup>C{<sup>1</sup>H} (bottom) NMR spectra of **16β** in CDCl<sub>3</sub>.
- Figure S16** <sup>1</sup>H (top) and <sup>13</sup>C{<sup>1</sup>H} (bottom) NMR spectra of **16α** in CDCl<sub>3</sub>.
- Figure S17** ESI mass spectrum of **3**.
- Figure S18** ESI mass spectrum of **4**.
- Figure S19** ESI mass spectrum of **6**.
- Figure S20** ESI mass spectrum of **9**.
- Figure S21** ESI mass spectrum of **10**.
- Figure S22** ESI mass spectrum of **11**.
- Figure S23** ESI mass spectrum of **14β**.
- Figure S24** ESI mass spectrum of **14α**.
- Figure S25** ESI mass spectrum of **15β**.
- Figure S26** ESI mass spectrum of **15α**.
- Figure S27** ESI mass spectrum of **16β**.
- Figure S28** ESI mass spectrum of **16α**.



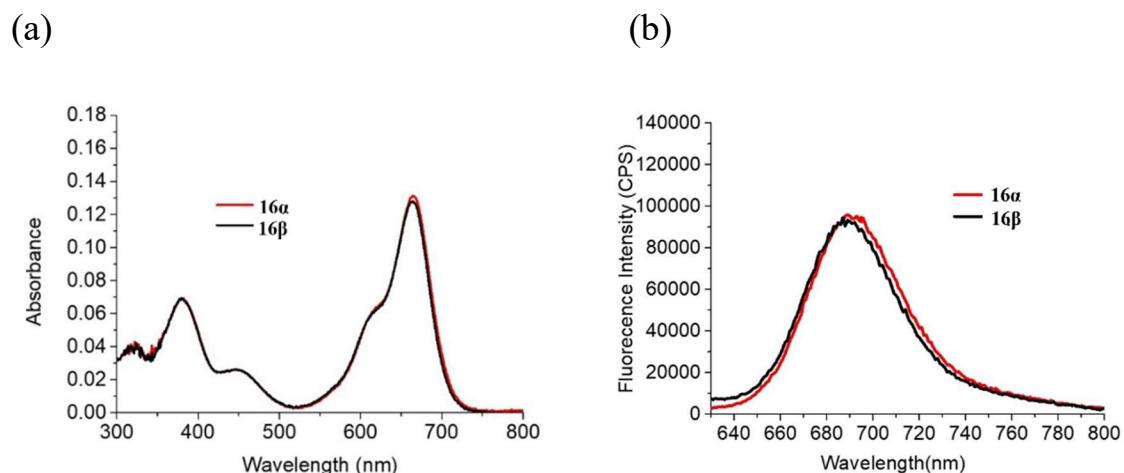
**Figure S1.** (a) Electronic absorption and (b) fluorescence (excited at 610 nm) spectra of **16α** and **16β** (both at 2  $\mu\text{M}$ ) in DMF.



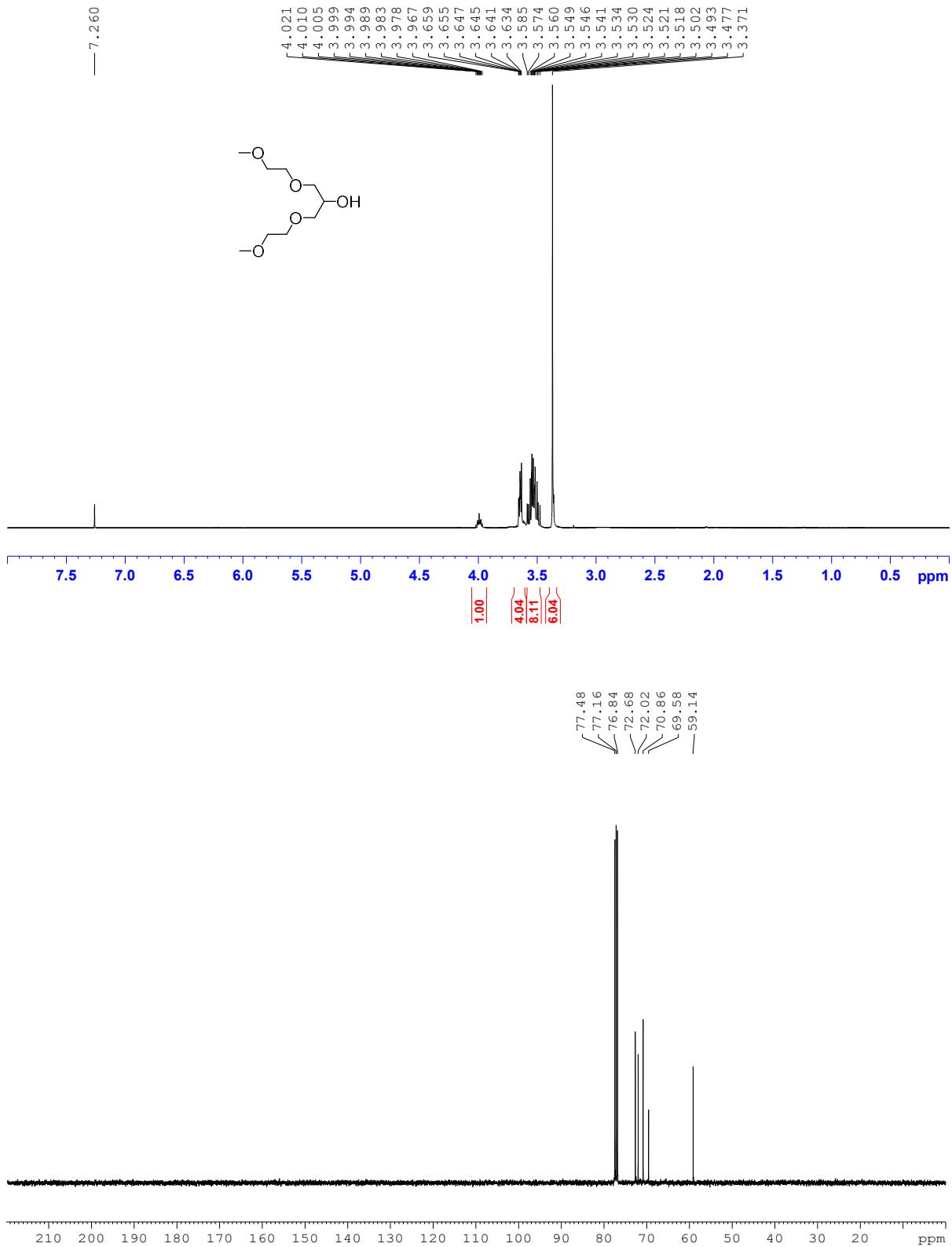
**Figure S2.** UV-Vis spectra of (a) **16α** and (b) **16β** at different concentrations in DMF. The inset of each figure plots the Q-band absorbance at 662 nm against the concentration of the dye.



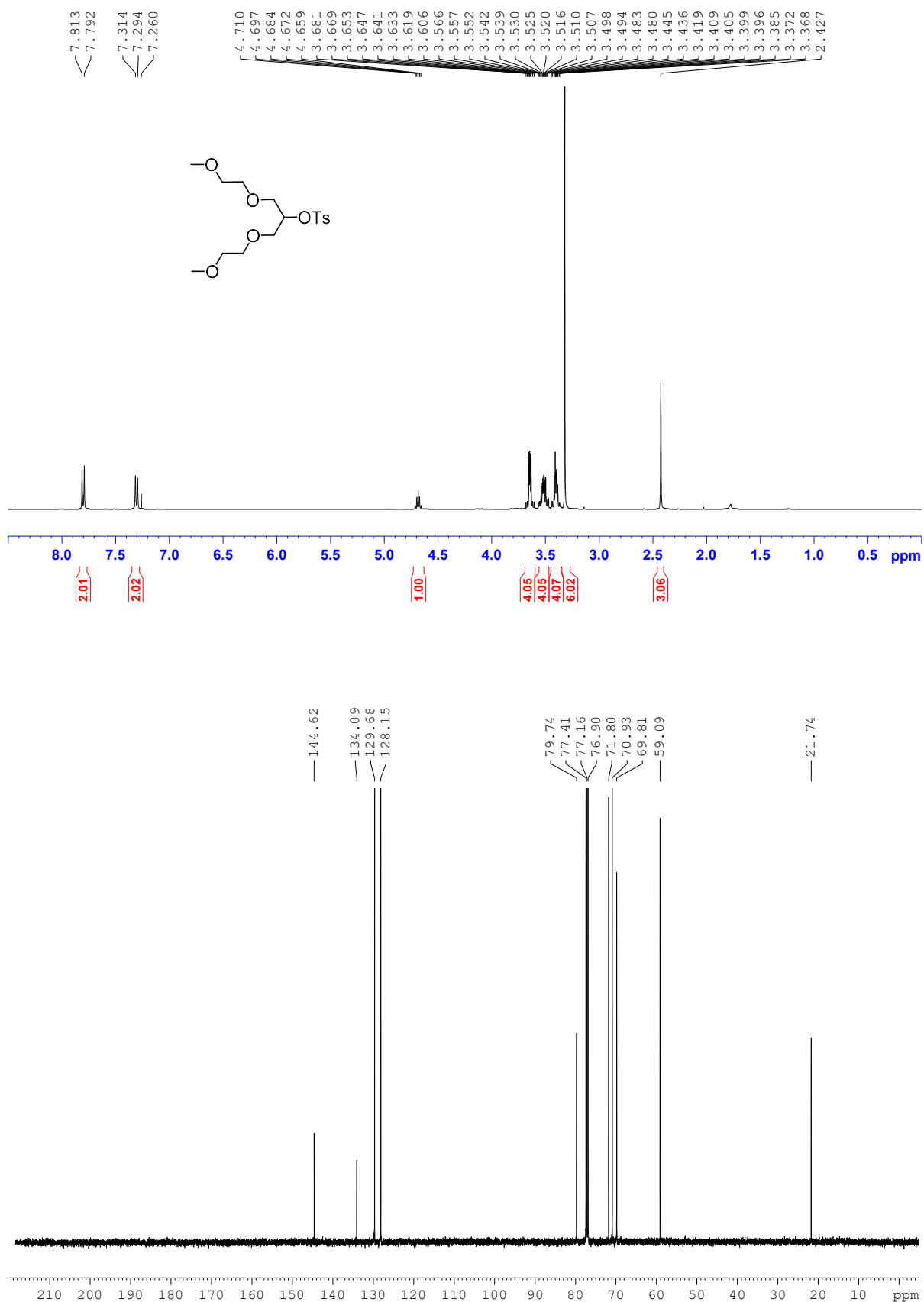
**Figure S3.** Comparison of the rate of photodecay of DPBF (initial concentration = 30  $\mu\text{M}$ ) in (a) DMF and (b) PBS (pH = 7.4) with 0.1% Tween 80 (v/v) using **16α**, **16β**, and ZnPc (all at 2  $\mu\text{M}$ ) as the photosensitizers.



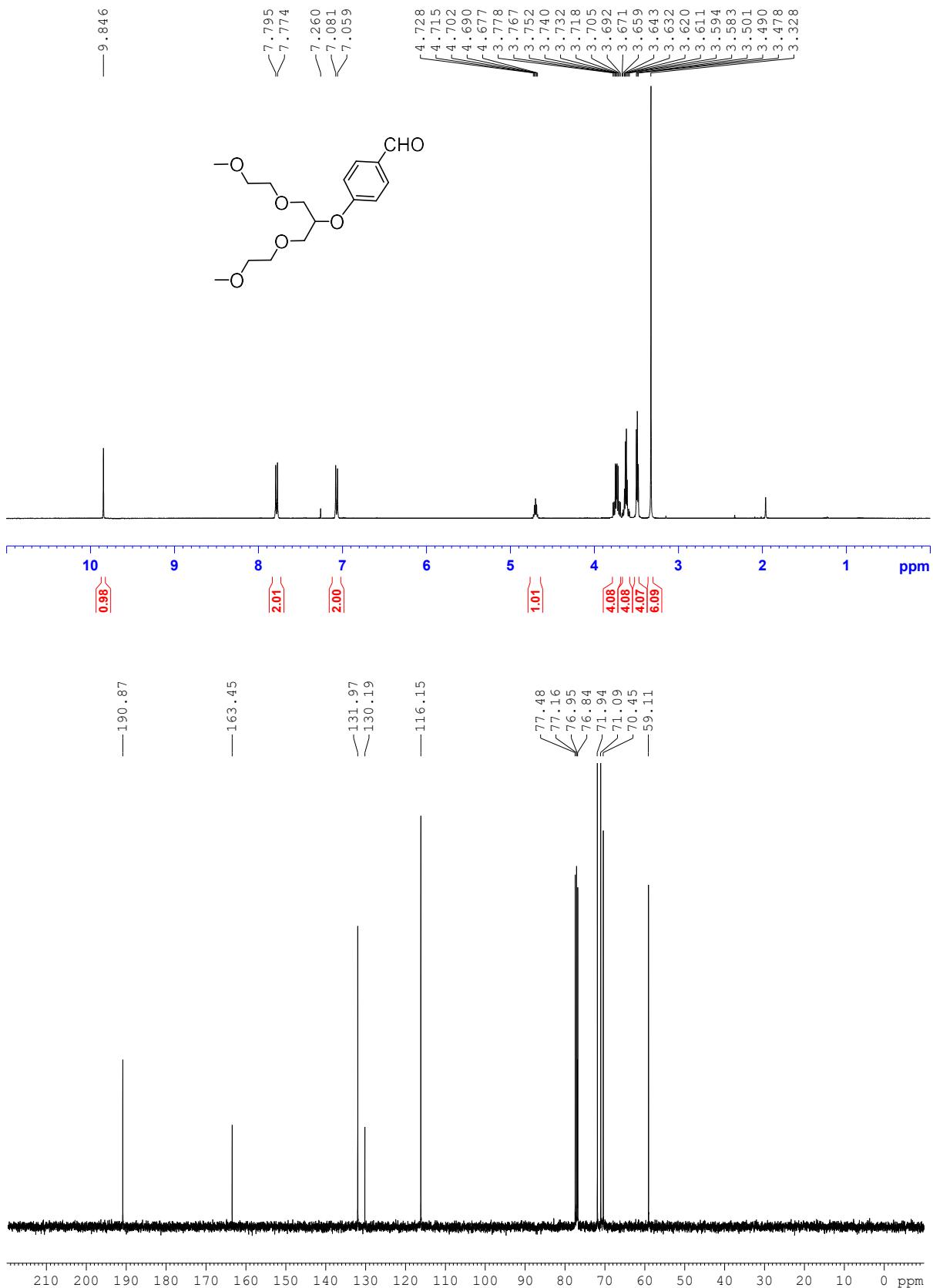
**Figure S4.** (a) Electronic absorption and (b) fluorescence (excited at 610 nm) spectra of **16α** and **16β** (both at 2  $\mu\text{M}$ ) in PBS (pH = 7.4) with 0.1% Tween 80 (v/v).



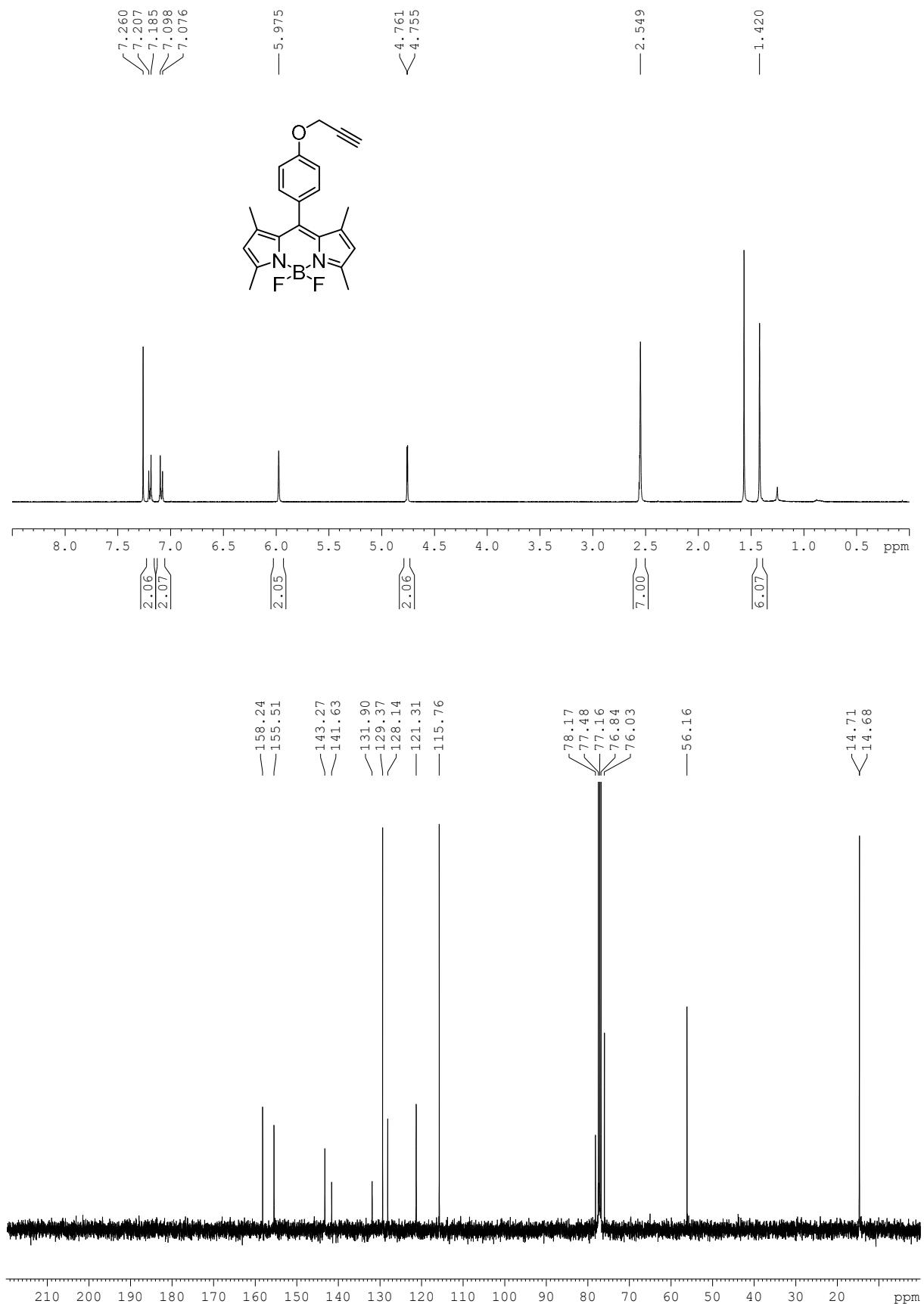
**Figure S5.** <sup>1</sup>H (top) and <sup>13</sup>C{<sup>1</sup>H} (bottom) NMR spectra of **3** in CDCl<sub>3</sub>.



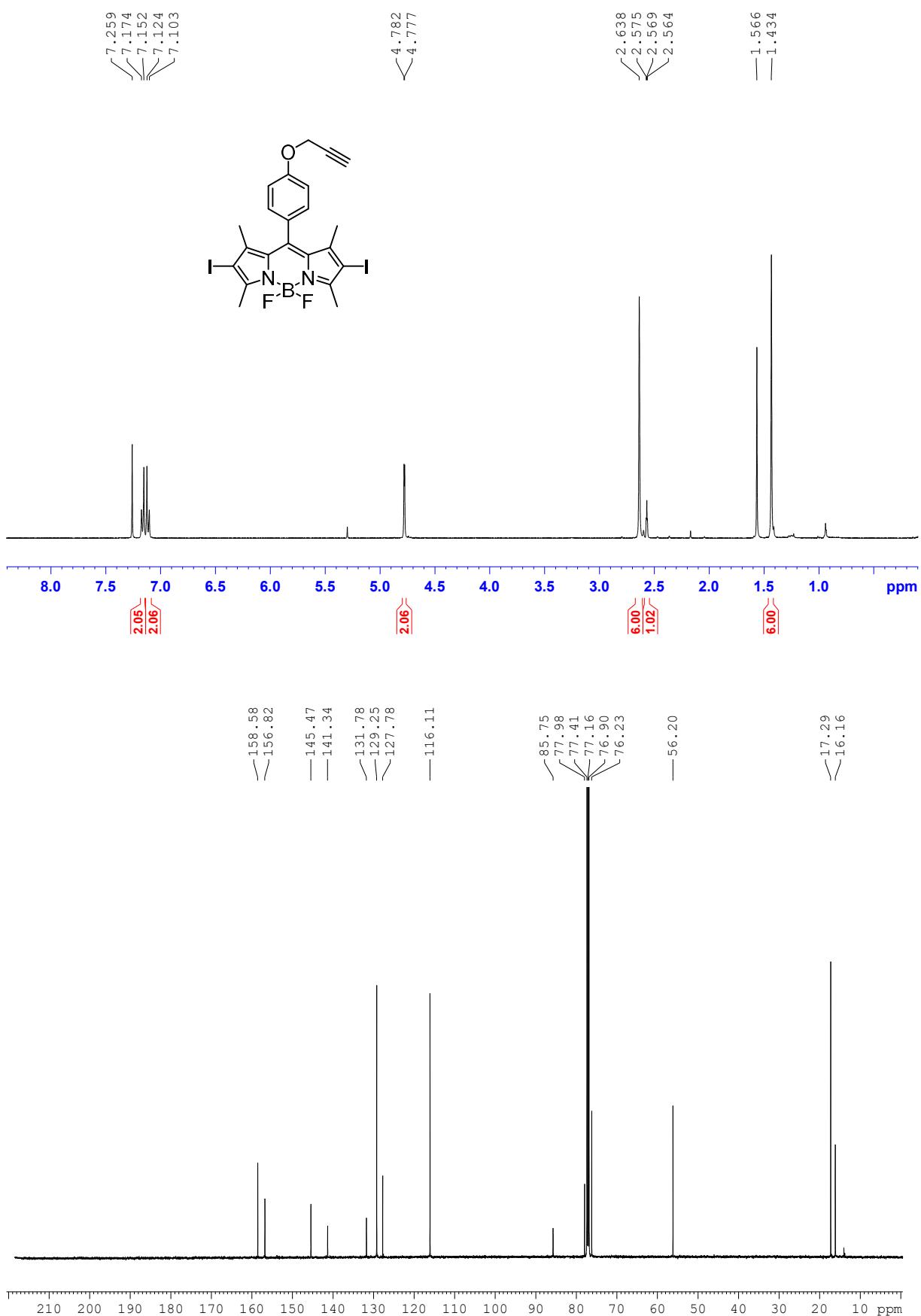
**Figure S6.**  $^1\text{H}$  (top) and  $^{13}\text{C}\{\text{H}\}$  (bottom) NMR spectra of **4** in  $\text{CDCl}_3$ .



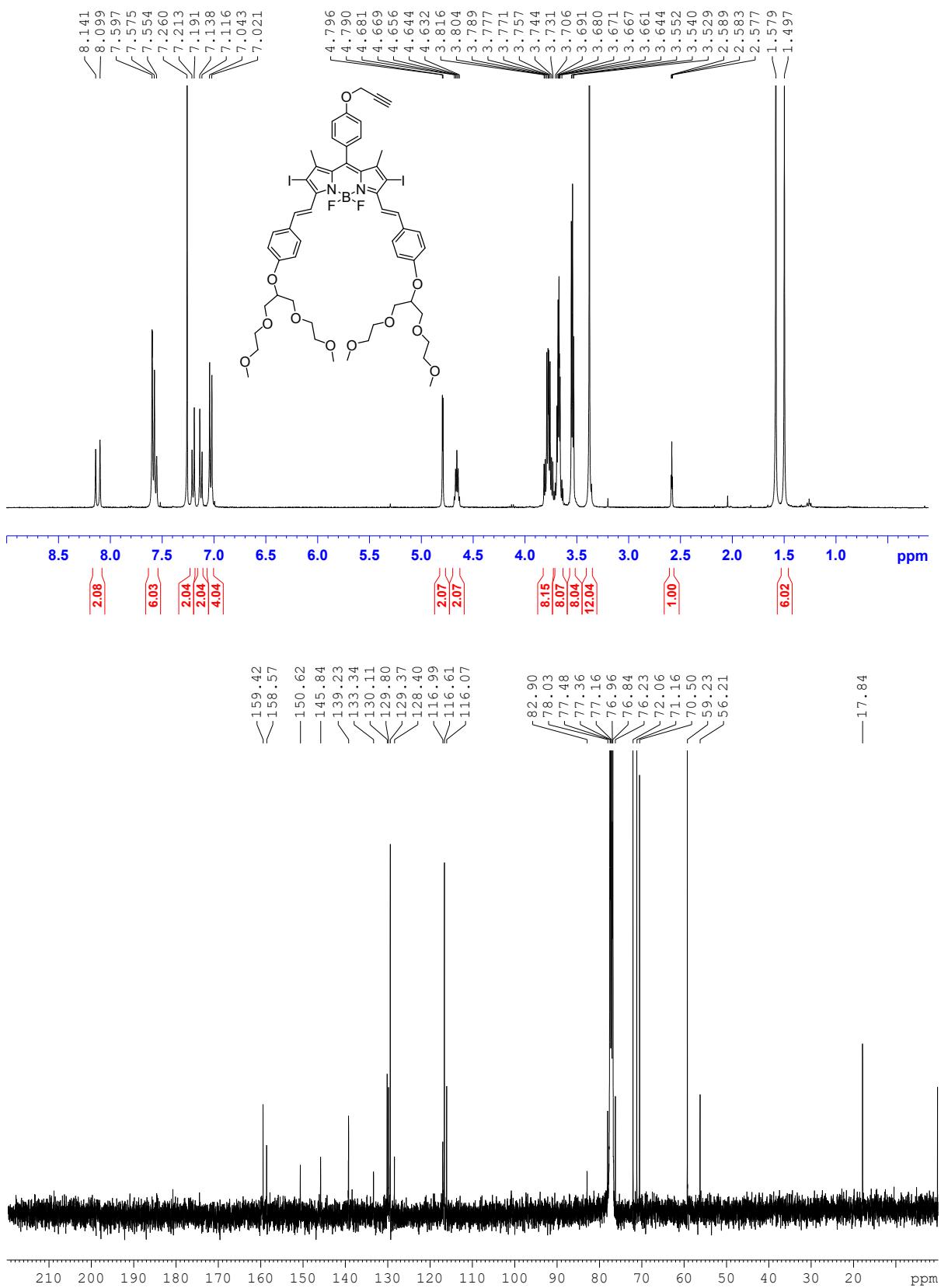
**Figure S7.**  $^1\text{H}$  (top) and  $^{13}\text{C}\{^1\text{H}\}$  (bottom) NMR spectra of **6** in CDCl<sub>3</sub>.



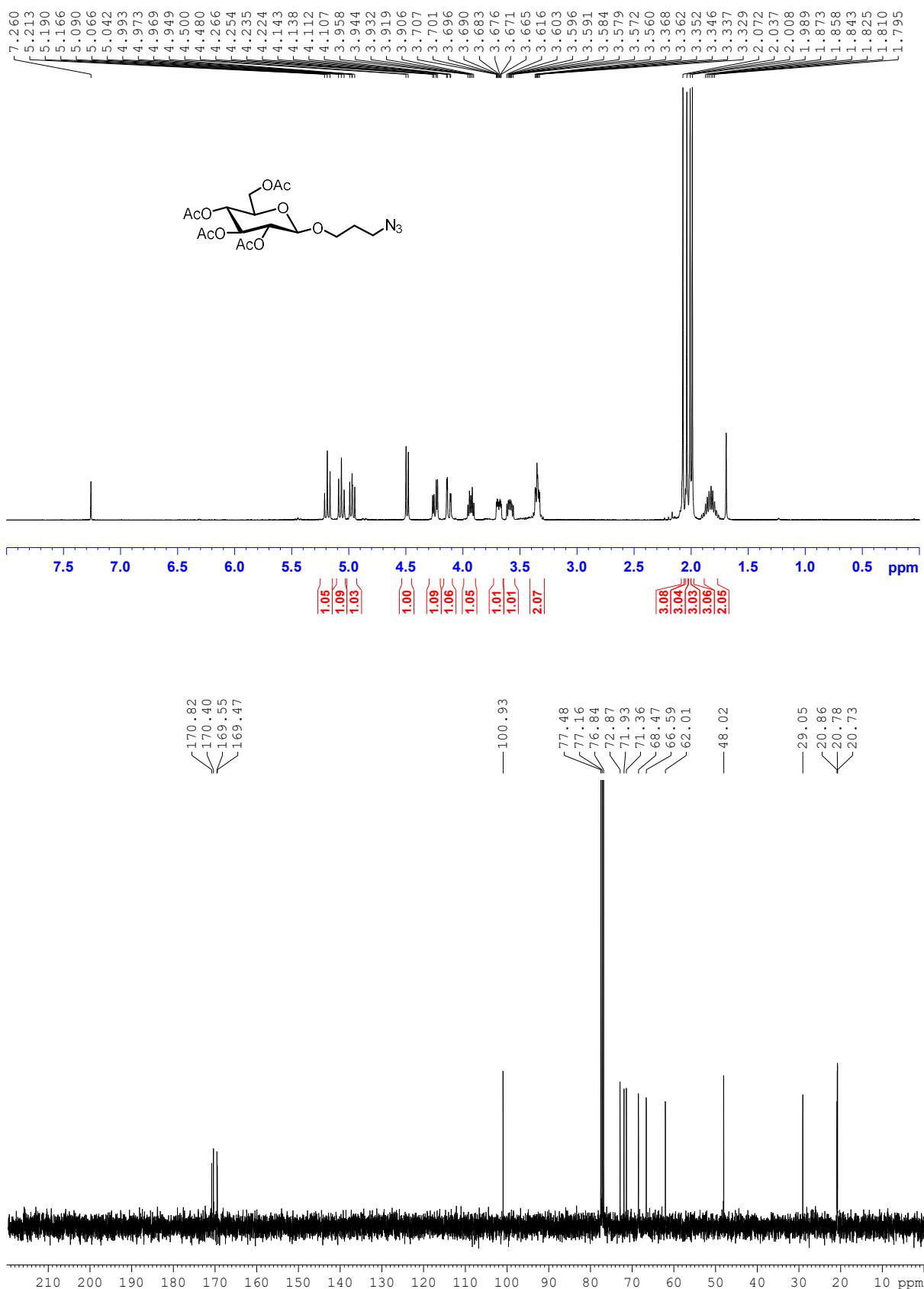
**Figure S8.**  $^1\text{H}$  (top) and  $^{13}\text{C}\{^1\text{H}\}$  (bottom) NMR spectra of **9** in  $\text{CDCl}_3$ .



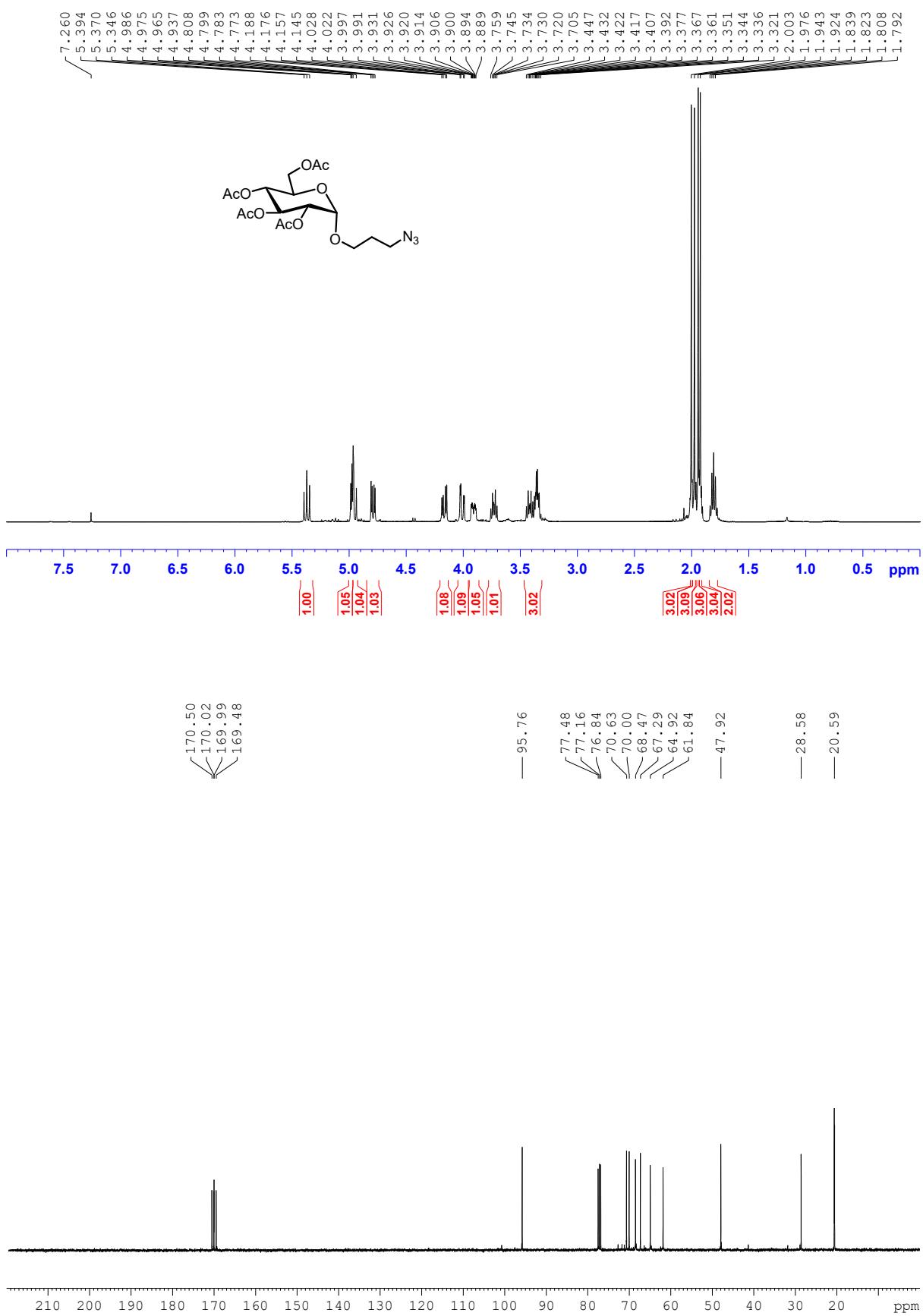
**Figure S9.**  $^1\text{H}$  (top) and  $^{13}\text{C}\{^1\text{H}\}$  (bottom) NMR spectra of **10** in  $\text{CDCl}_3$ .



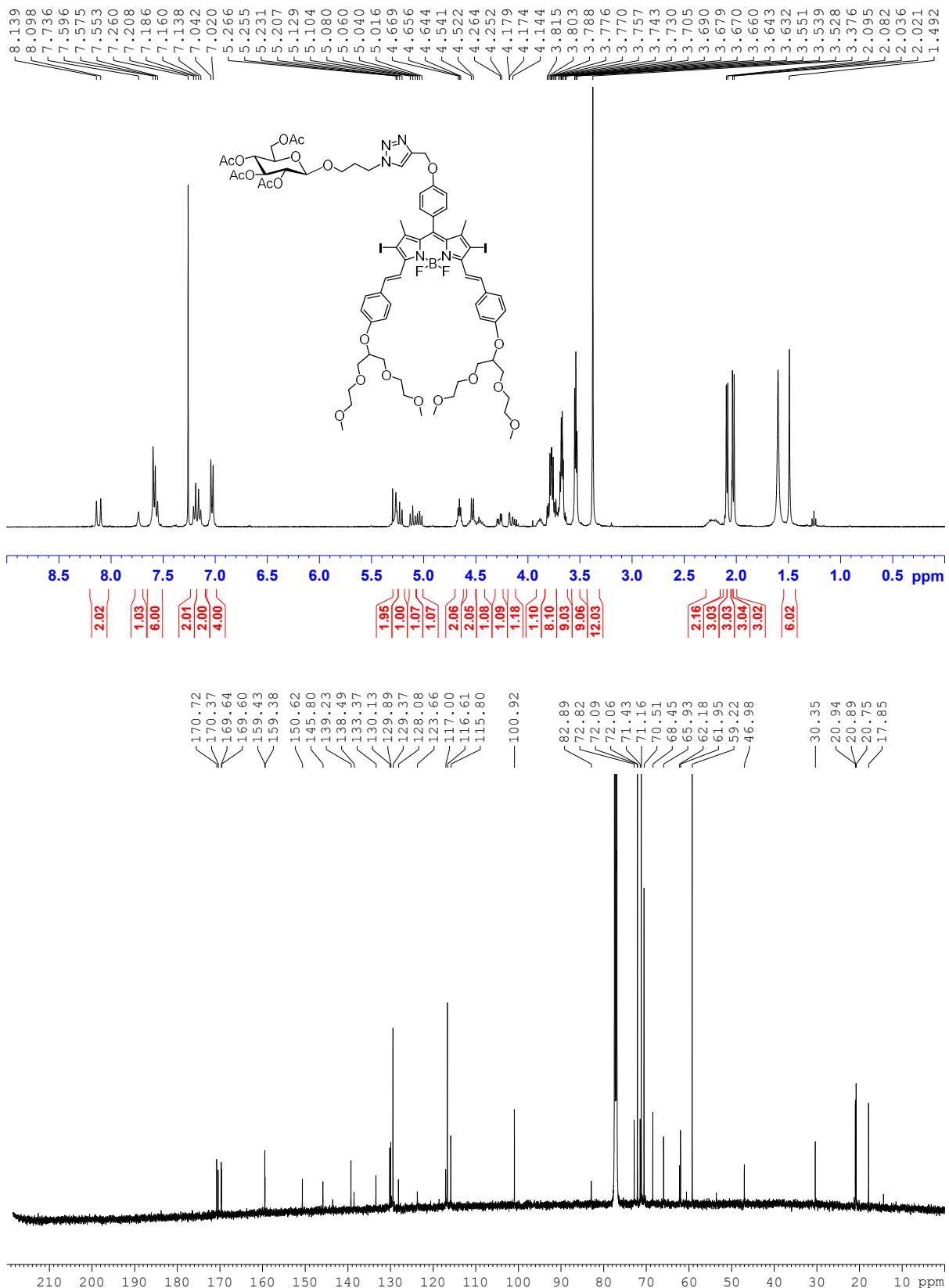
**Figure S10.**  $^1\text{H}$  (top) and  $^{13}\text{C}\{^1\text{H}\}$  (bottom) NMR spectra of **11** in  $\text{CDCl}_3$ .



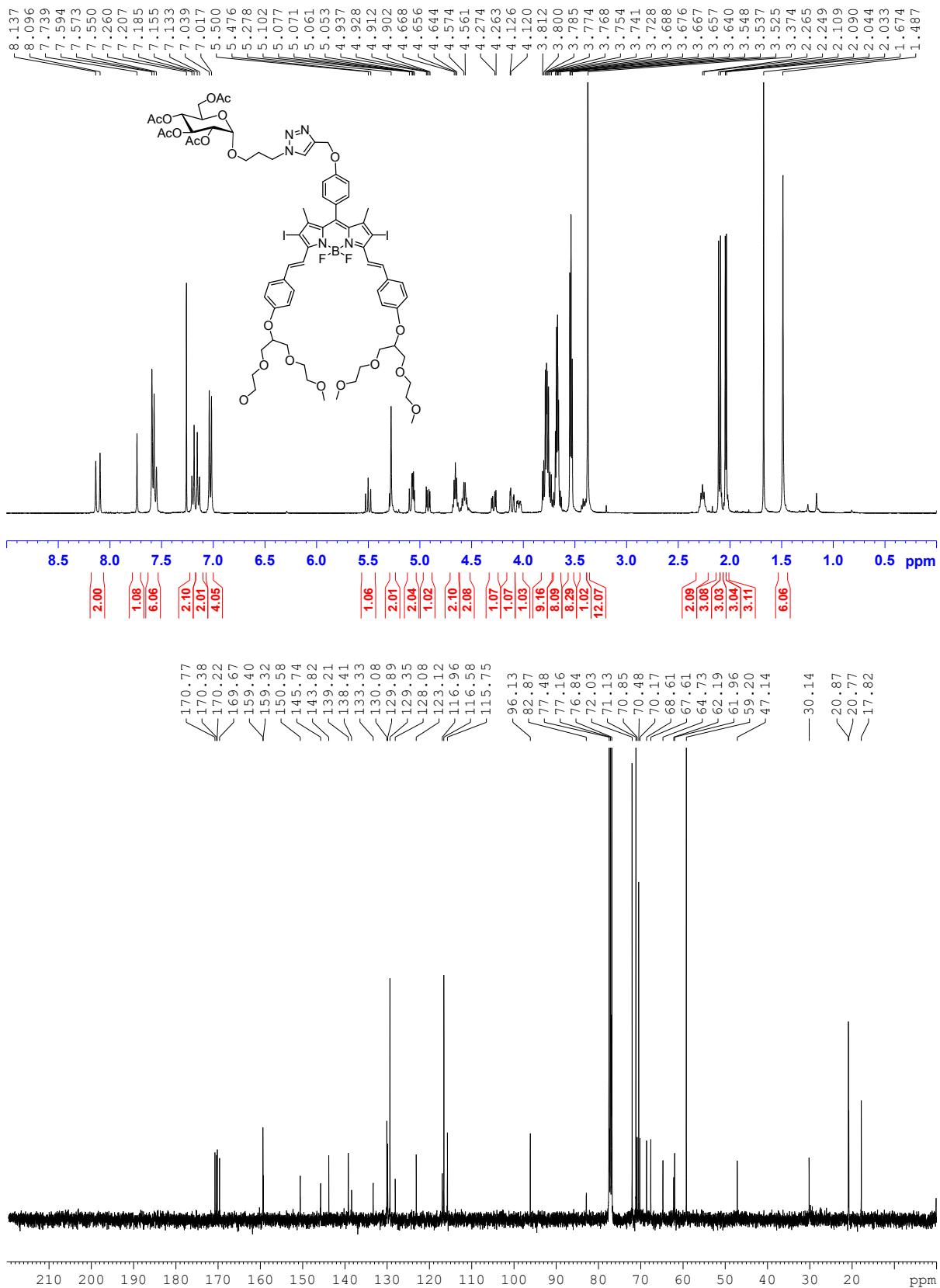
**Figure S11.**  $^1\text{H}$  (top) and  $^{13}\text{C}\{\text{H}\}$  (bottom) NMR spectra of **14 $\beta$**  in  $\text{CDCl}_3$ .



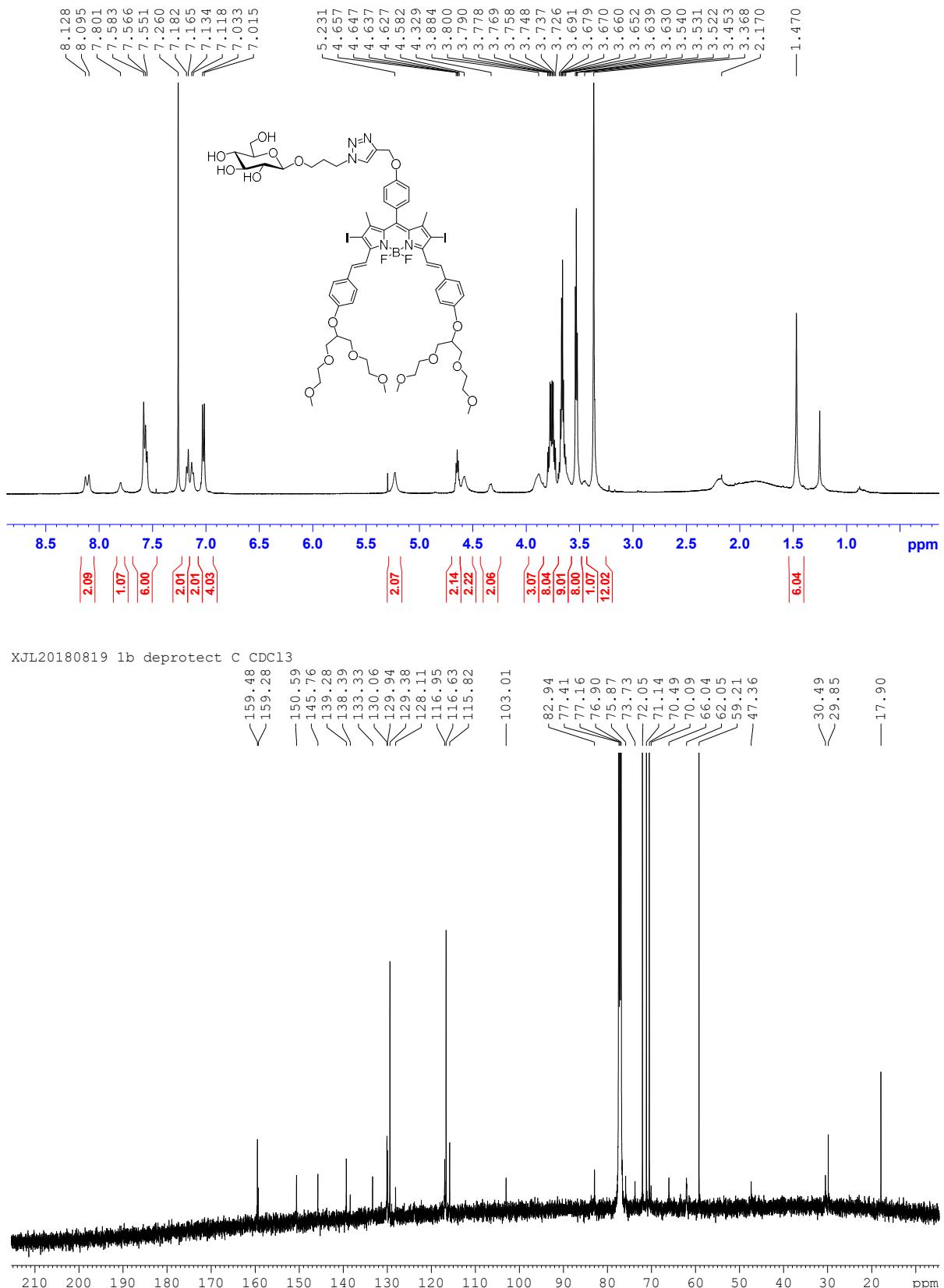
**Figure S12.**  $^1\text{H}$  (top) and  $^{13}\text{C}\{^1\text{H}\}$  (bottom) NMR spectra of **14a** in CDCl<sub>3</sub>.



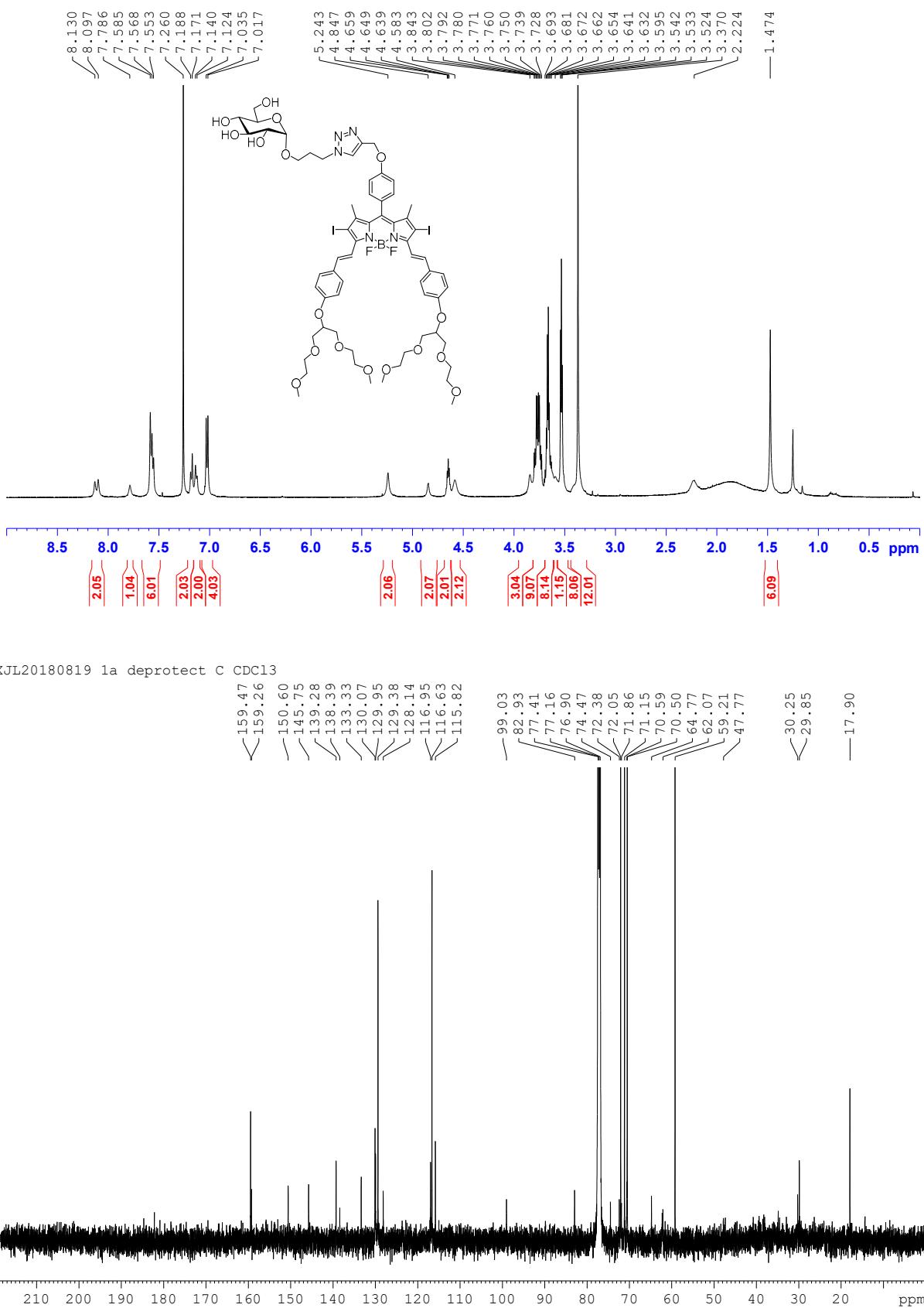
**Figure S13.**  $^1\text{H}$  (top) and  $^{13}\text{C}\{^1\text{H}\}$  (bottom) NMR spectra of  $\mathbf{15\beta}$  in  $\text{CDCl}_3$ .



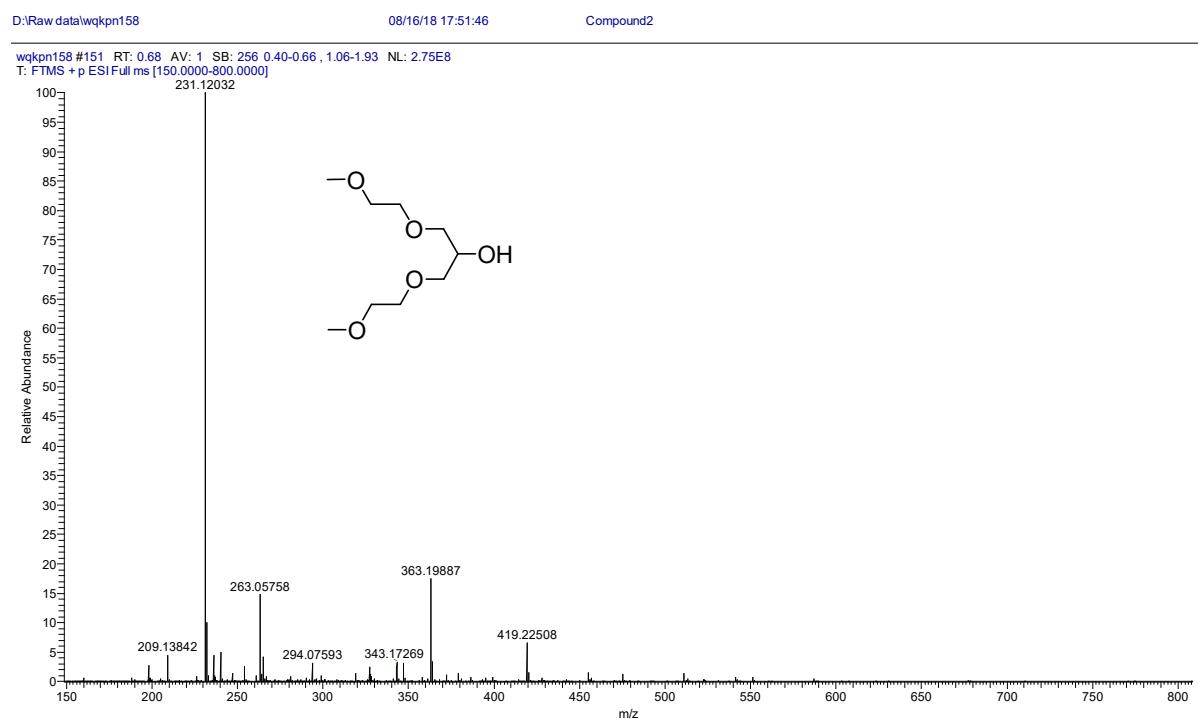
**Figure S14.**  $^1\text{H}$  (top) and  $^{13}\text{C}\{^1\text{H}\}$  (bottom) NMR spectra of **15a** in  $\text{CDCl}_3$ .



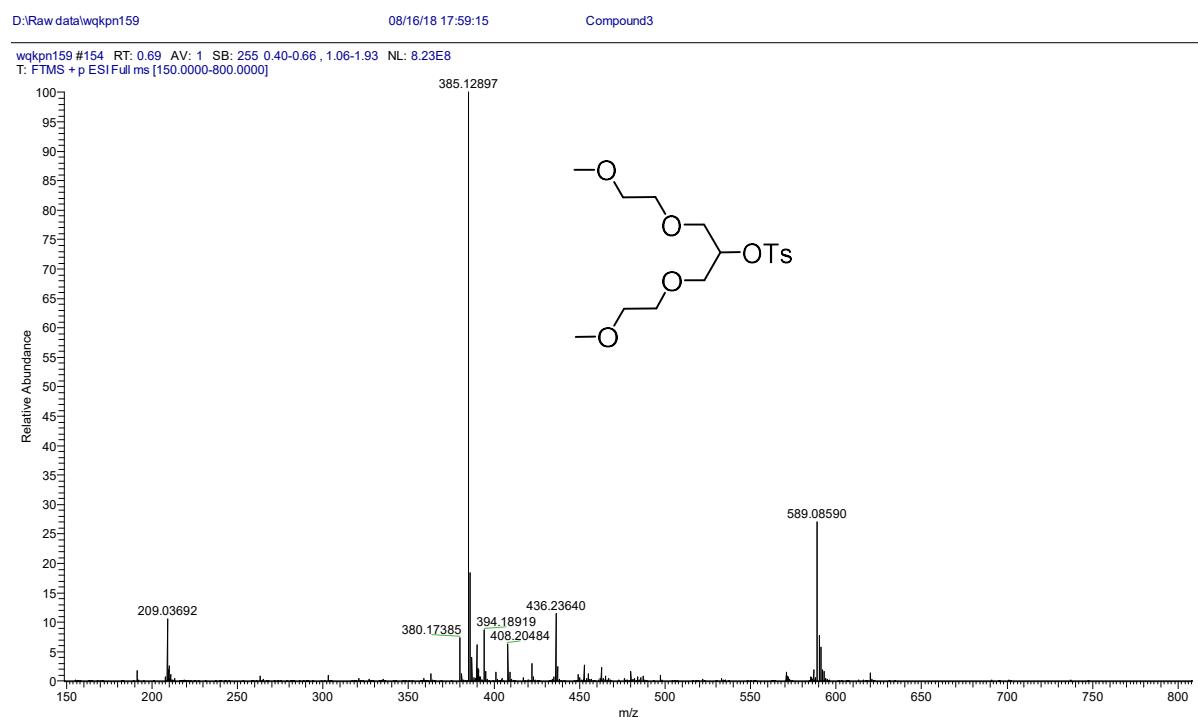
**Figure S15.**  $^1\text{H}$  (top) and  $^{13}\text{C}\{^1\text{H}\}$  (bottom) NMR spectra of **16 $\beta$**  in  $\text{CDCl}_3$ .



**Figure S16.**  $^1\text{H}$  (top) and  $^{13}\text{C}\{^1\text{H}\}$  (bottom) NMR spectra of **16a** in  $\text{CDCl}_3$ .

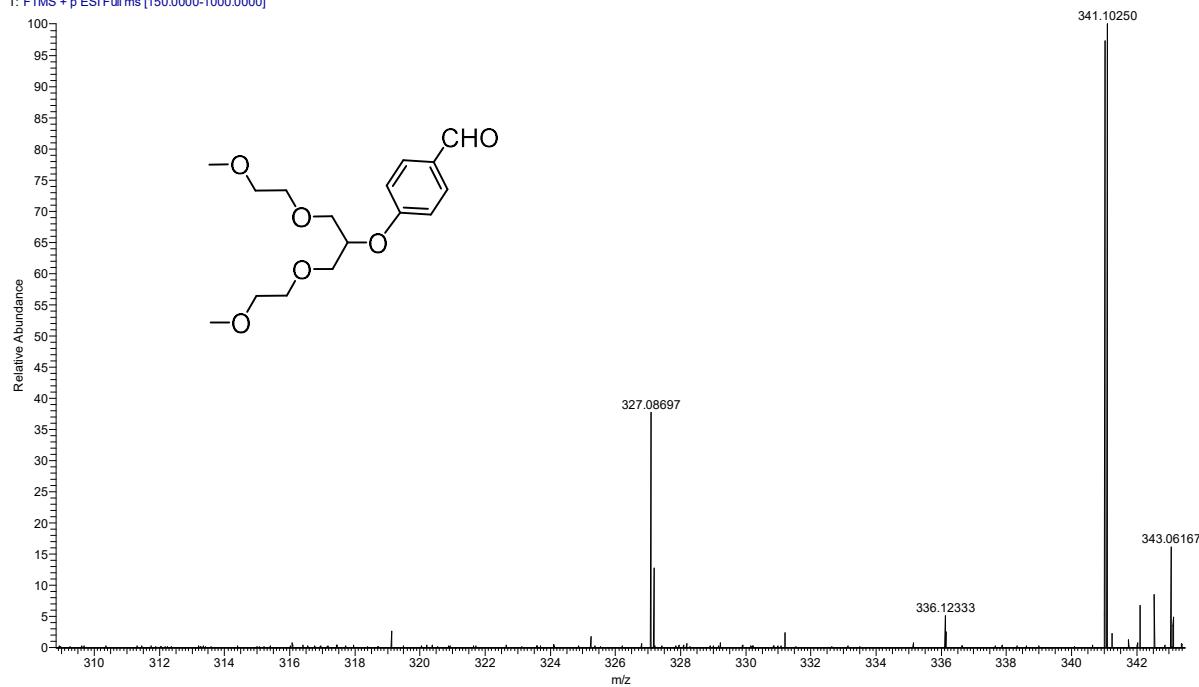


**Figure S17.** ESI mass spectrum of 3.



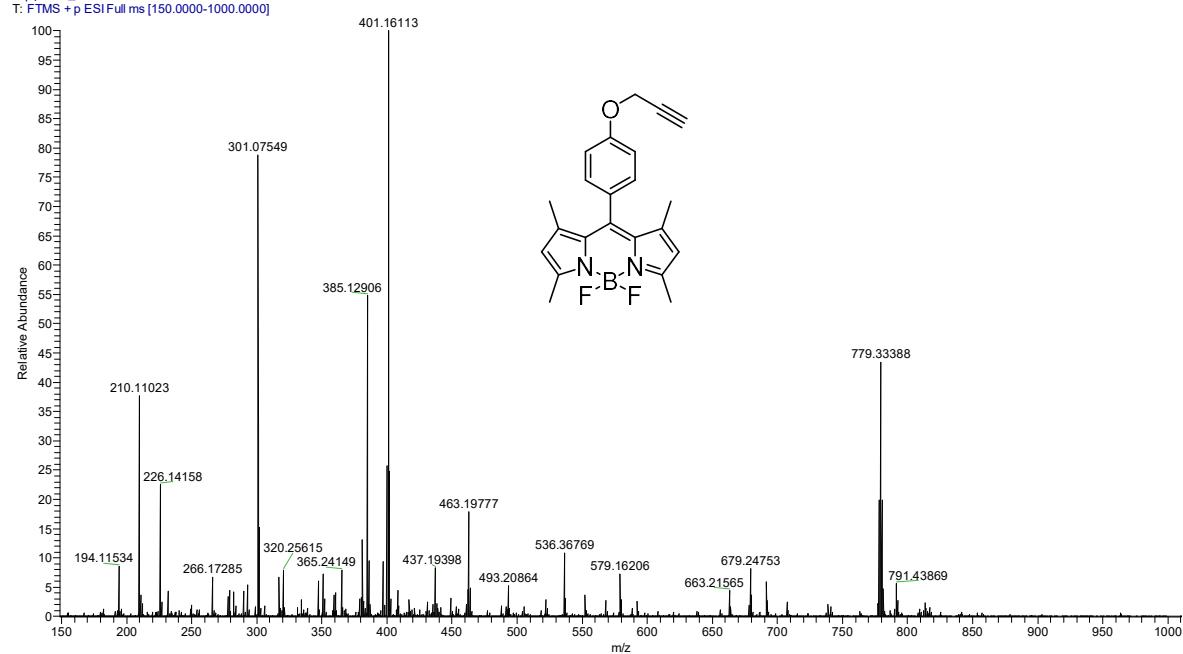
**Figure S18.** ESI mass spectrum of 4.

wqkpn160\_180817104853 #478-556 RT: 2.13-2.48 AV: 79 SB: 83 0.00-0.37 NL: 1.60E6  
T: FTMS + p ESI Full ms [150.0000-1000.0000]

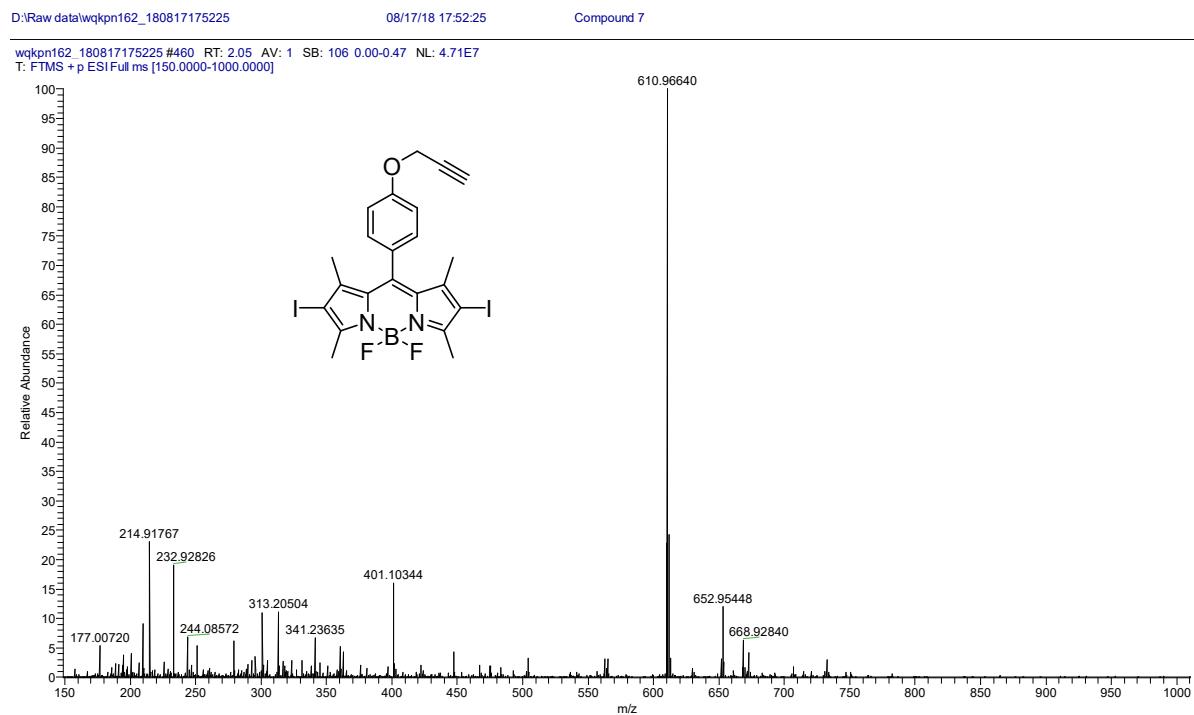


**Figure S19.** ESI mass spectrum of 6.

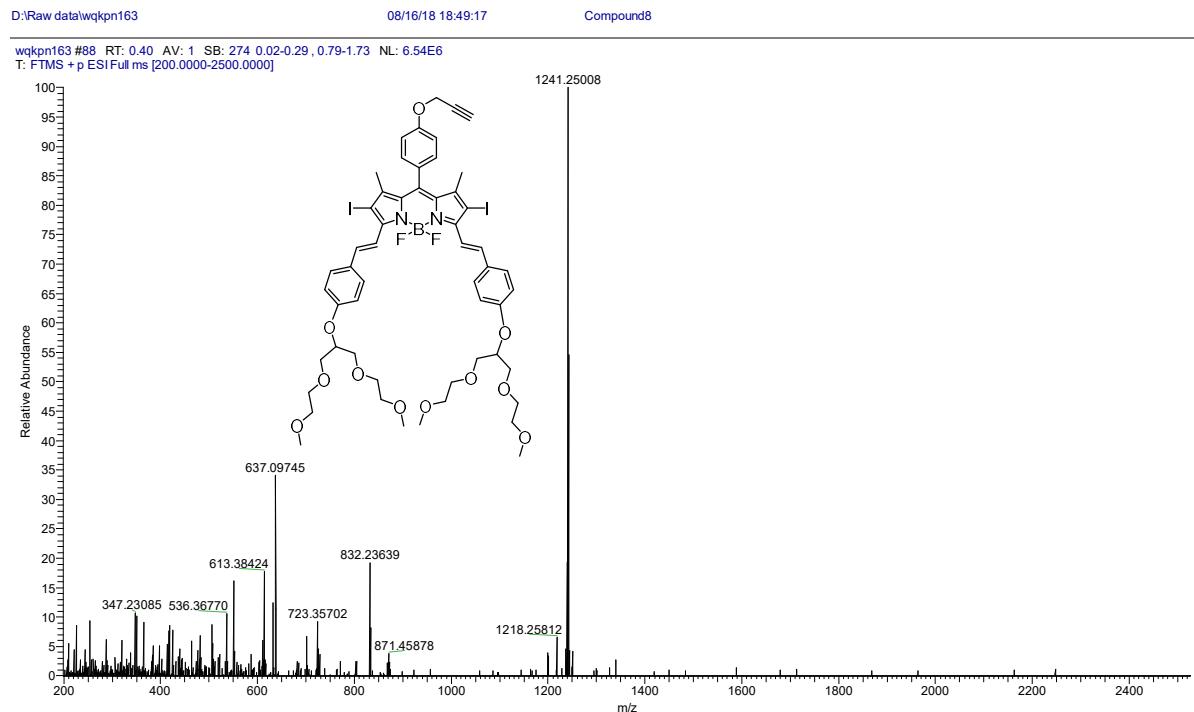
D:\Raw data\wqkpn161\_180817113555 08/17/18 11:35:55 Compound 6



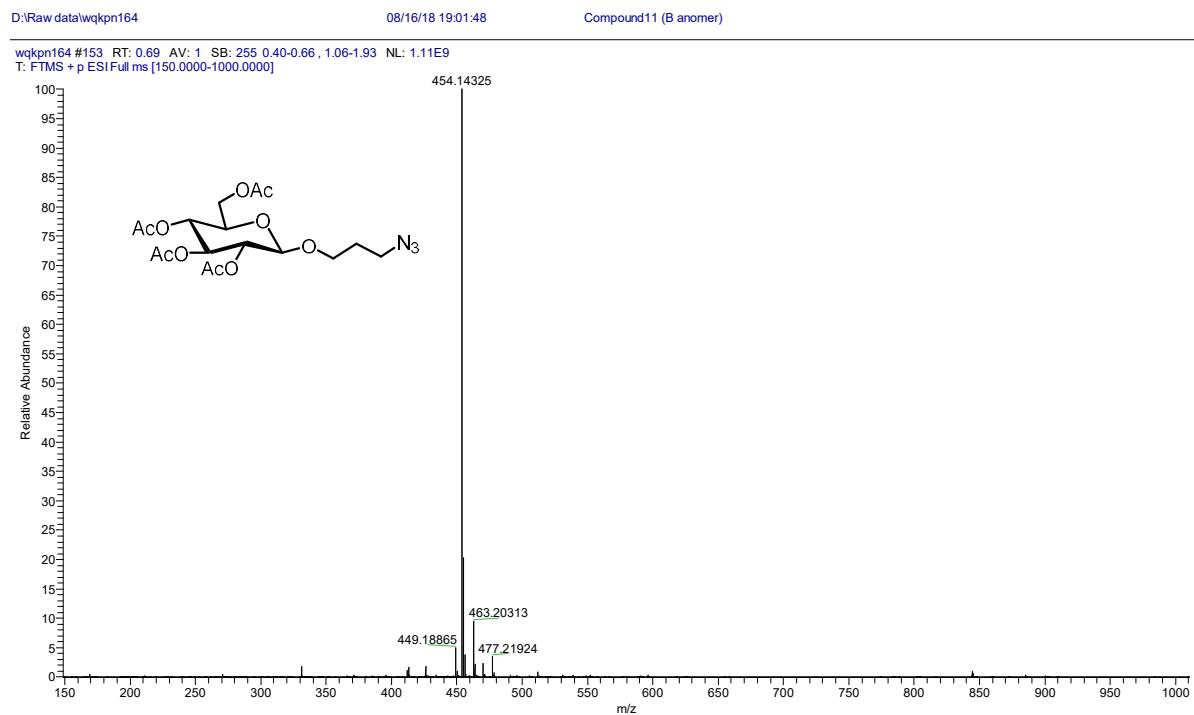
**Figure S20.** ESI mass spectrum of 9.



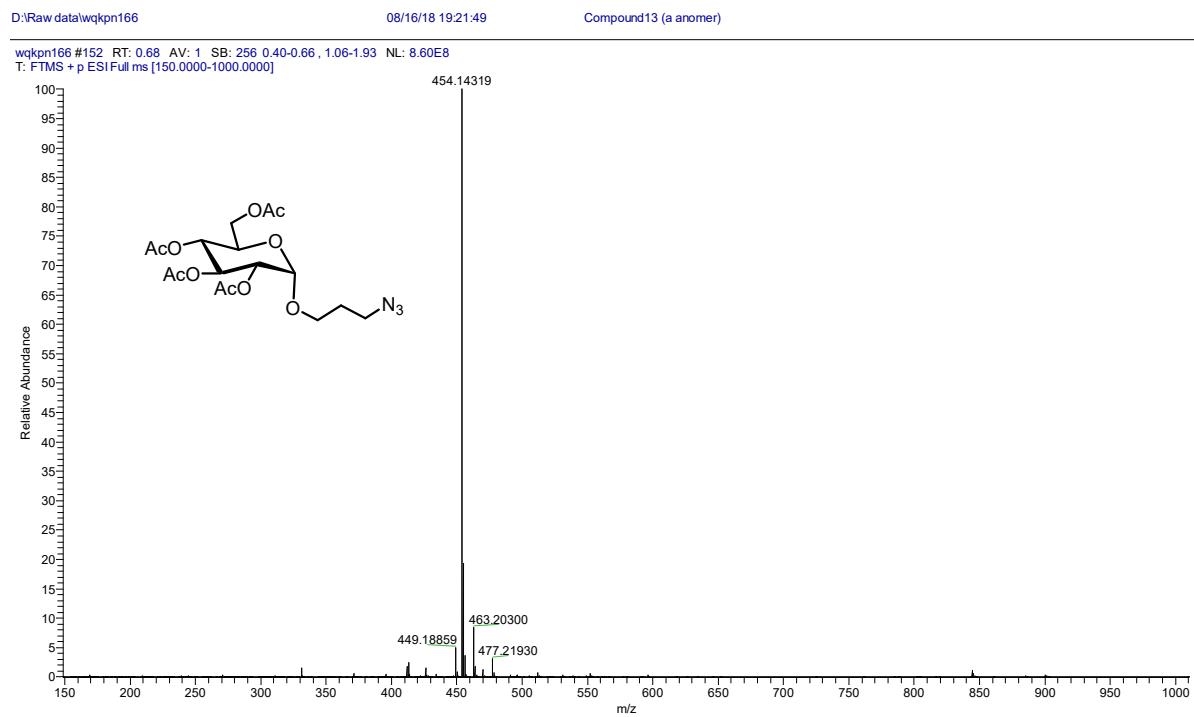
**Figure S21.** ESI mass spectrum of **10**.



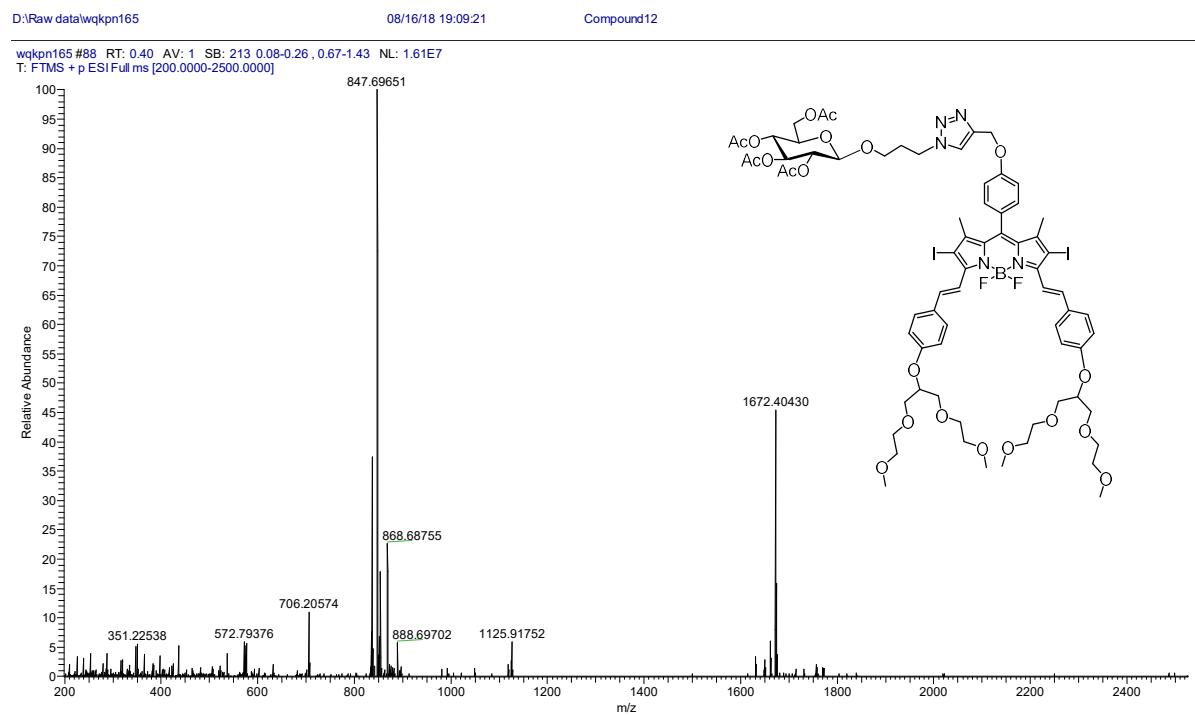
**Figure S22.** ESI mass spectrum of **11**.



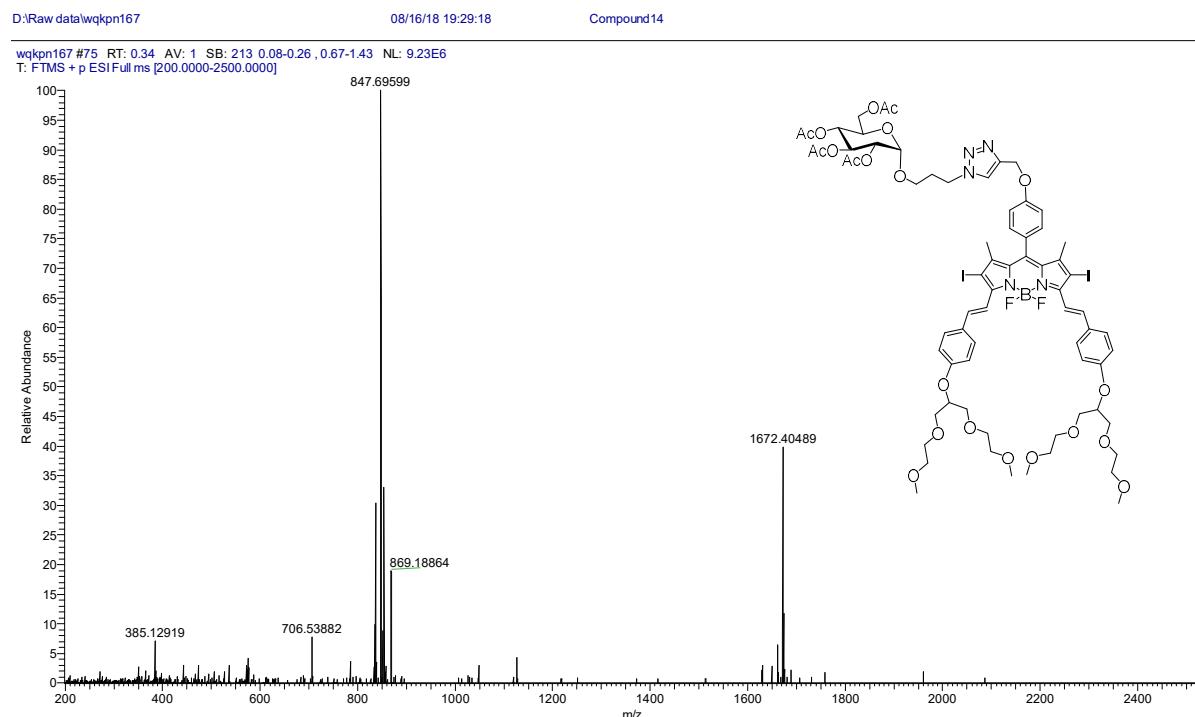
**Figure S23.** ESI mass spectrum of **14 $\beta$** .



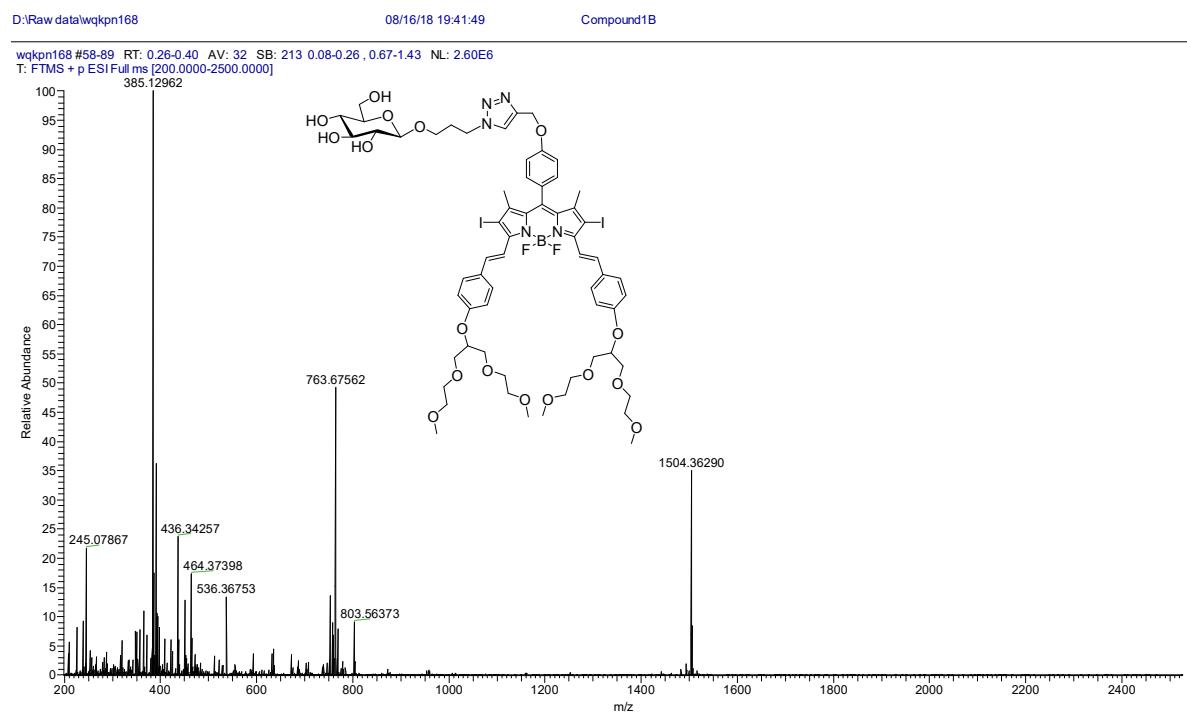
**Figure S24.** ESI mass spectrum of **14 $\alpha$** .



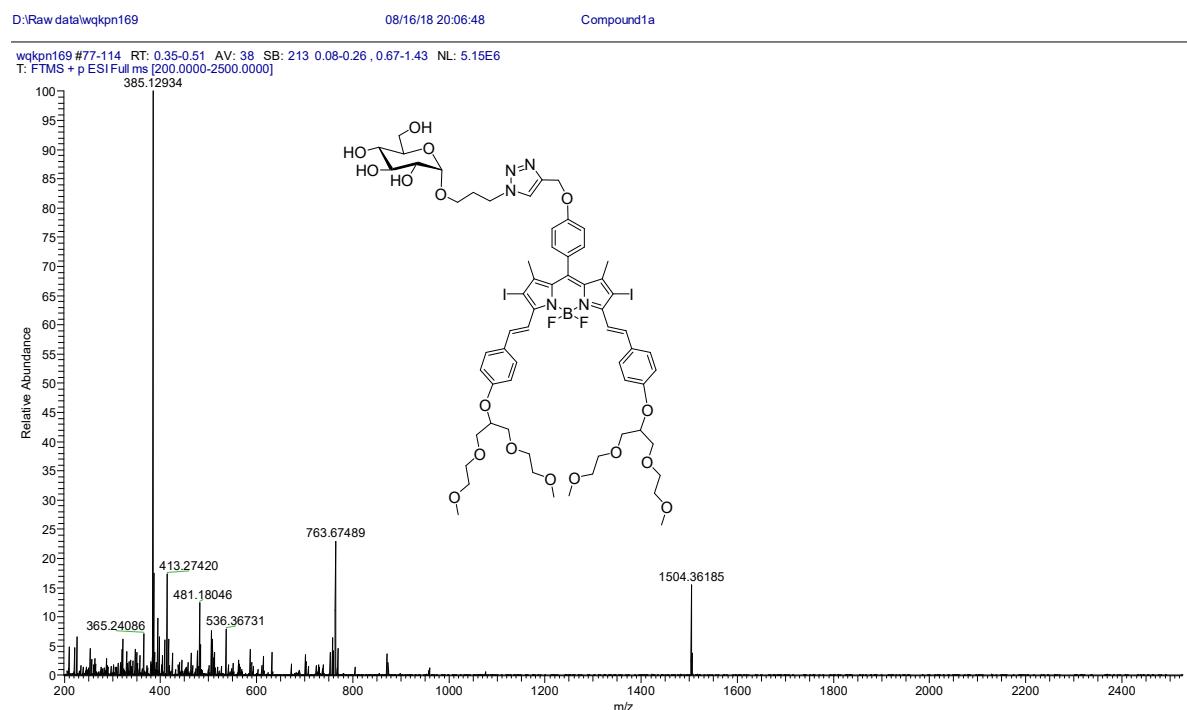
**Figure S25.** ESI mass spectrum of **15 $\beta$** .



**Figure S26.** ESI mass spectrum of **15 $\alpha$** .



**Figure S27.** ESI mass spectrum of **16 $\beta$** .



**Figure S28.** ESI mass spectrum of **16 $\alpha$** .