

Supporting Information

Mitochondrion-Targeting PEGylated BODIPY Dyes for Near-Infrared Cell Imaging and Photodynamic Therapy

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I. Concentration-dependent fluorescence intensity spectra

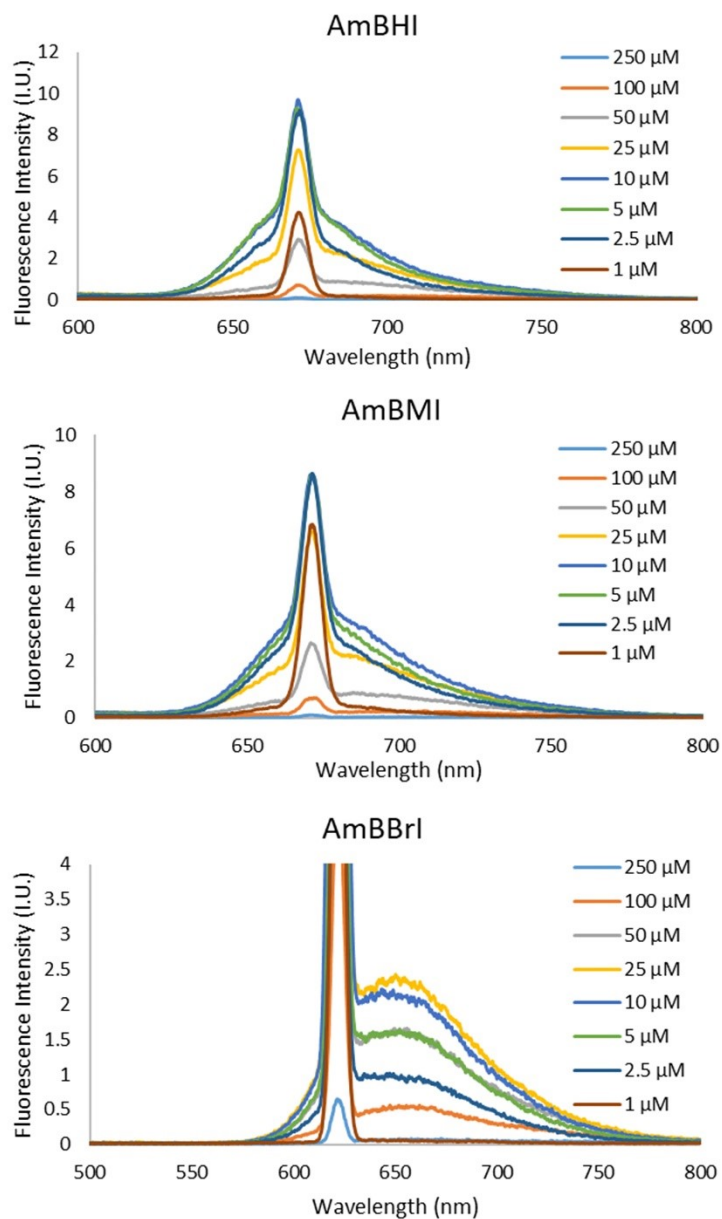


Figure S1. Concentration-dependent emission spectra of AmbXI dyes dissolved in water taken at room temperature. The excitation wavelength used was 662 nm for AmbBHI and AmbBMI and 612 nm for AmbBBrI.

II. Singlet oxygen generation efficiency in aqueous media

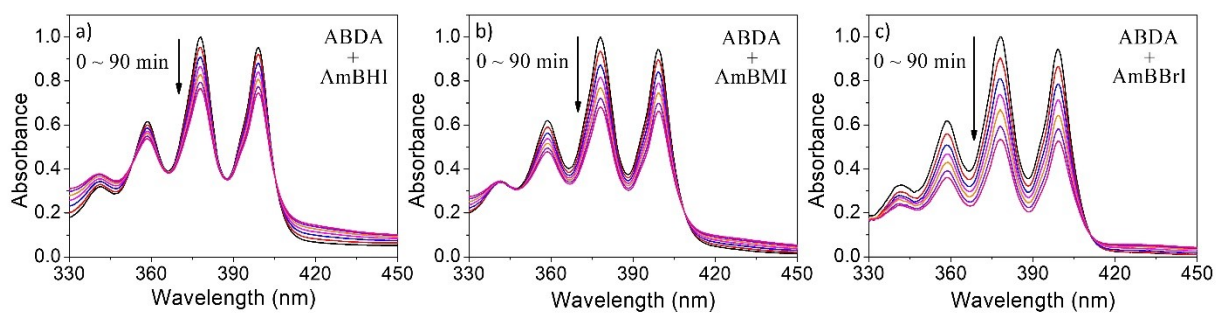


Figure S2. Singlet oxygen generation in aqueous media. Time-dependent absorption spectra of air-saturated water solutions of ABDA containing a) Δ MBHI, b) Δ MBMI, and c) AmBBrl under irradiation of 660 nm LED light.

III. Optimized structures of AmBXI

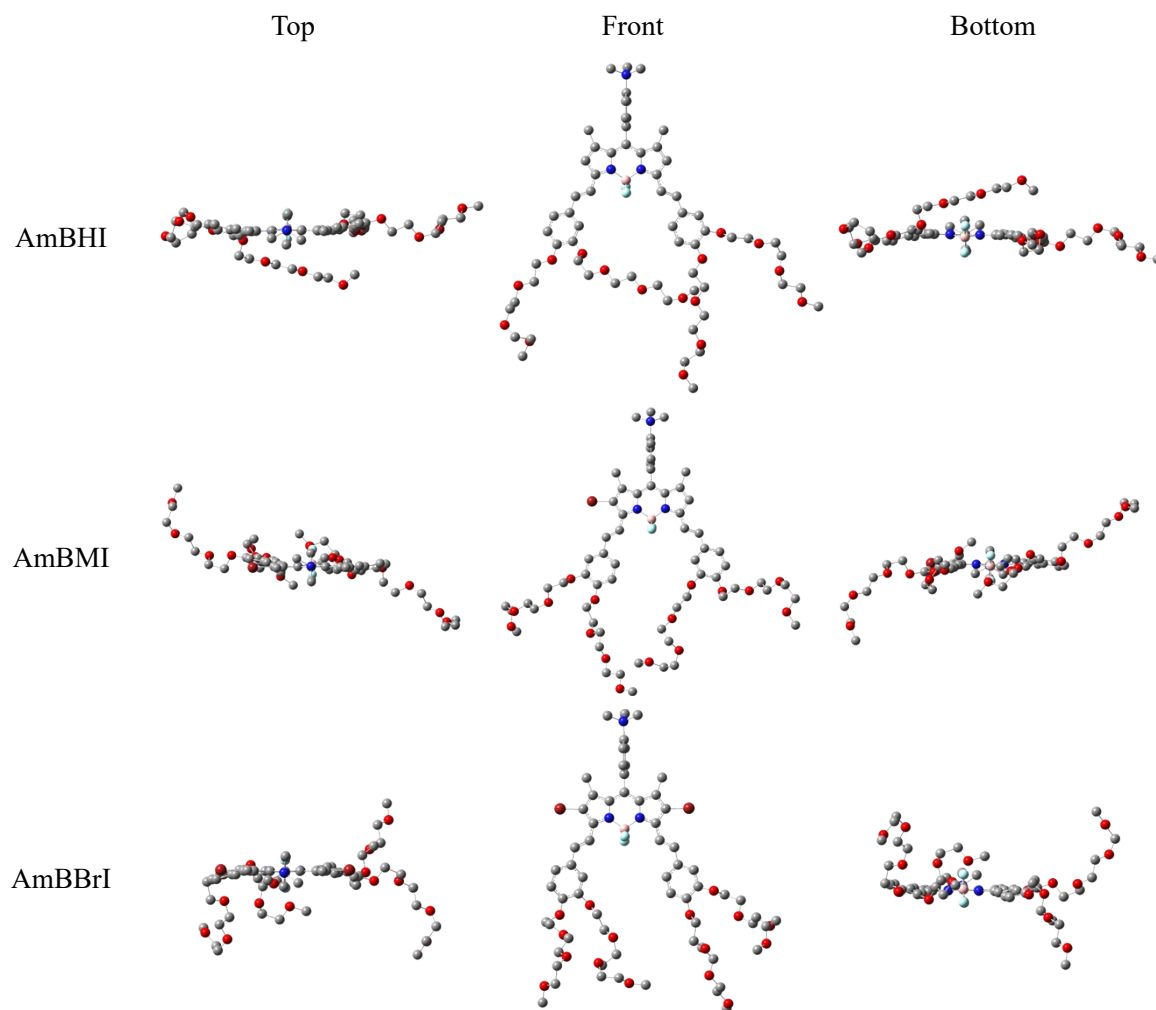


Figure S3. The optimized geometry of complete structures of BODIPY dyes. To clarify the optimized structures, hydrogen atoms are not shown in Figure. The coplanarity of the BODIPY core and the styryl group was confirmed through the three viewpoints: Top view (Left), Front view (middle), Bottom view (Right).

IV. Effects of AmBXI on apoptosis in cancer cells

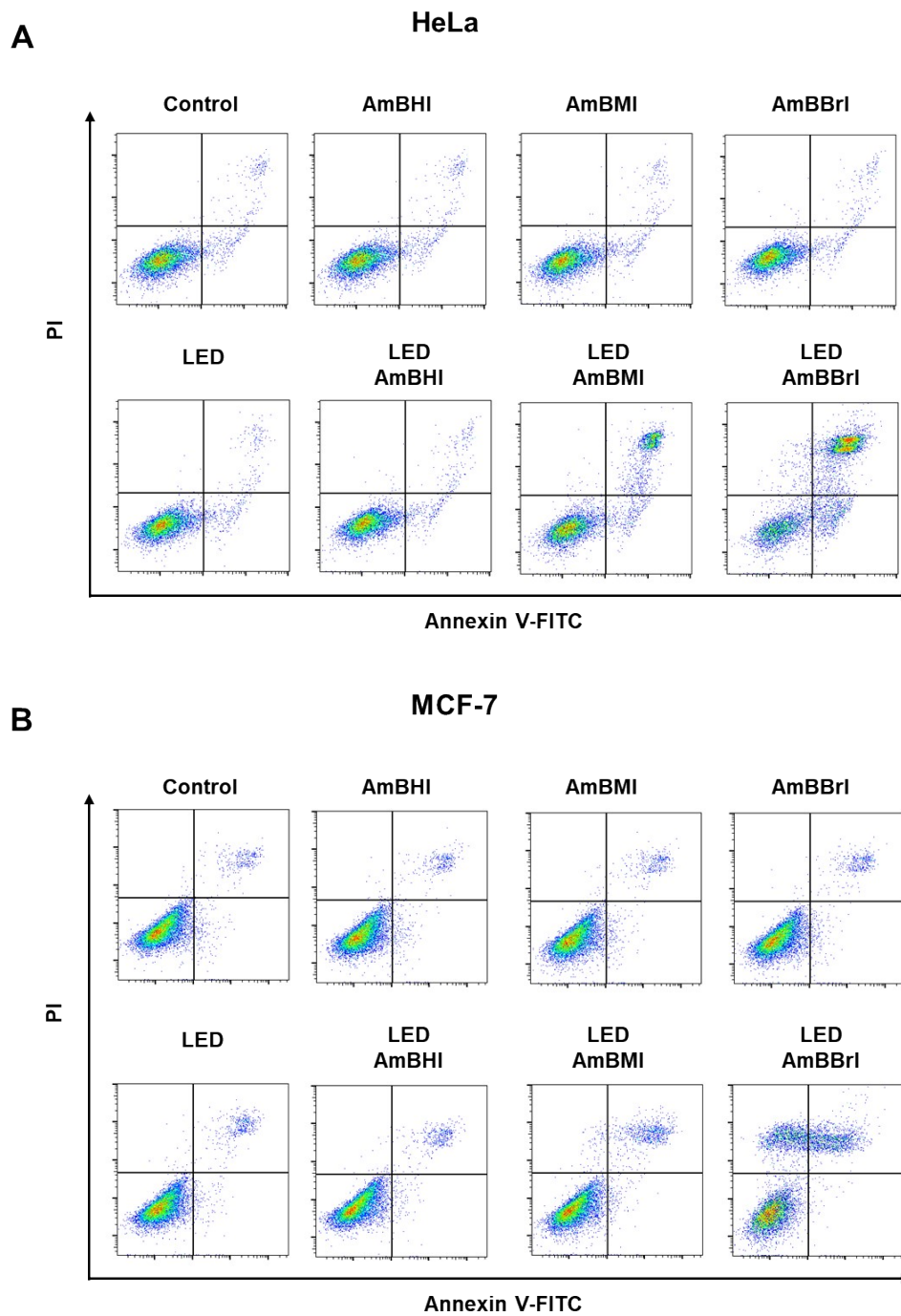


Figure S4. Effects of AmBXI on apoptosis in cancer cells.

V. Spectra

1. AmBDP (1)

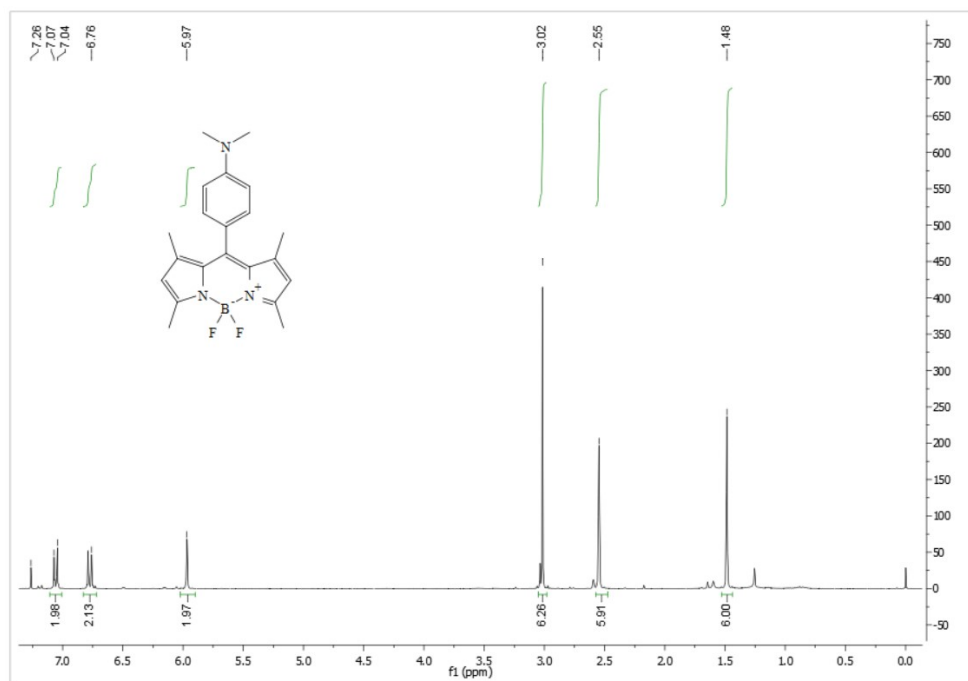


Figure S5. The ^1H NMR spectrum of AmBDP (1).

2. MonobromoAmBDP (2)

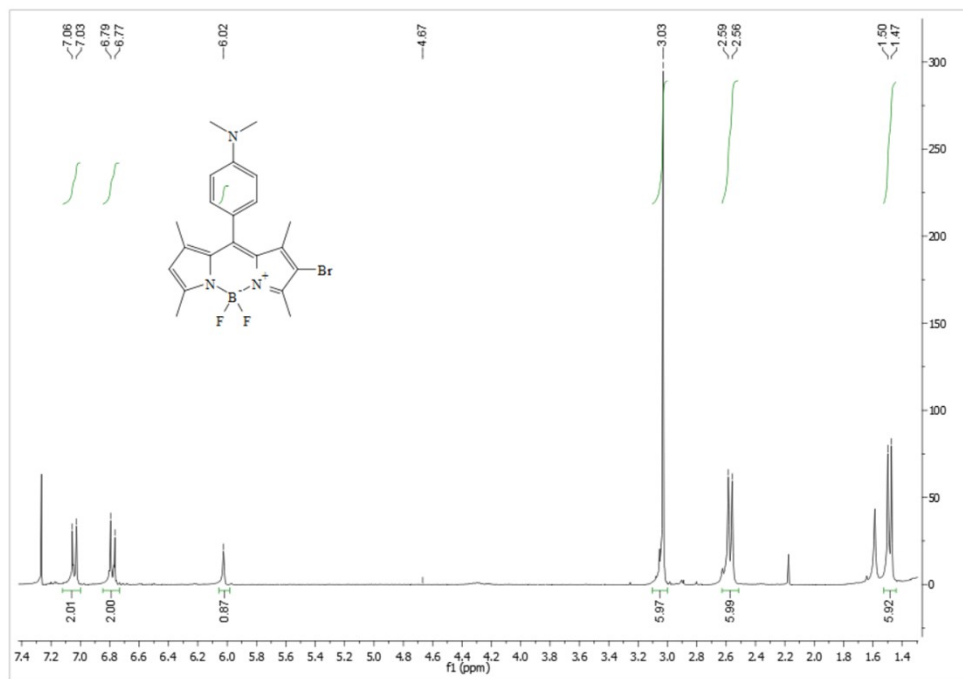


Figure S6. The ¹H NMR spectrum of monobromoAmBDP (2).

3. DibromoAmBDP (3)

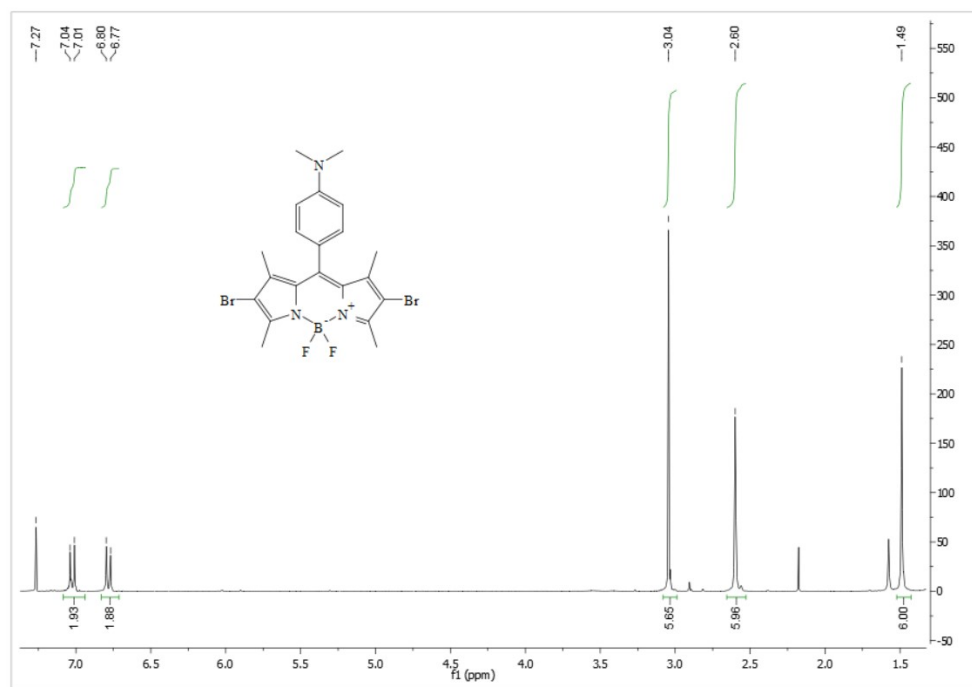


Figure S7. The ¹H NMR spectrum of dibromoAmBDP (3).

4. Tosyl-triethylene glycol

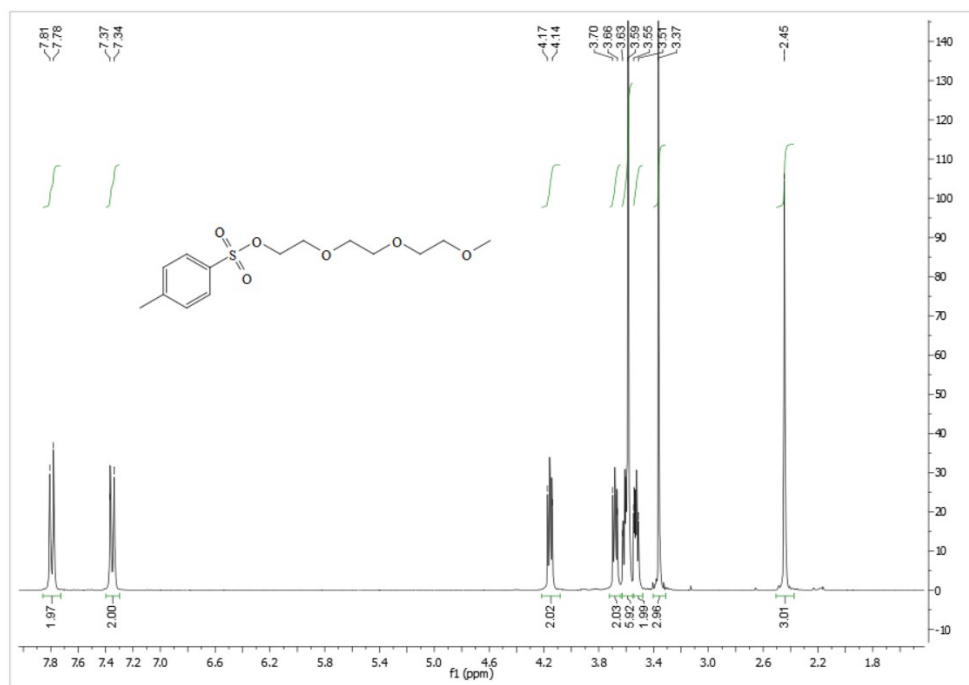


Figure S8. The ^1H NMR spectrum of tosyl-triethylene glycol.

5. 3,4-(ditriethylene glycol) carboxaldehyde (**4**)

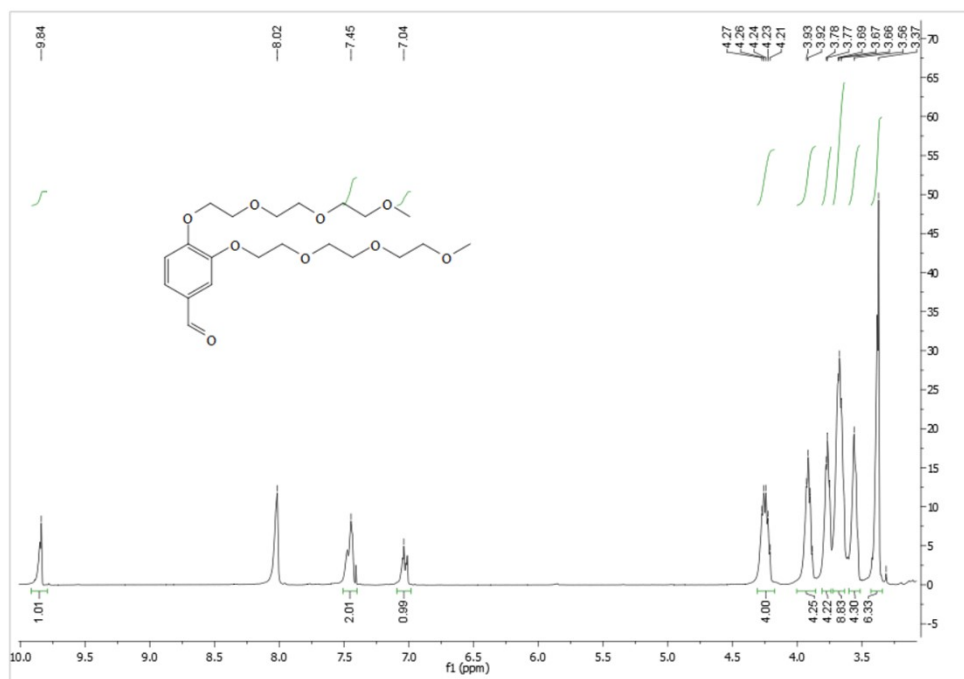


Figure S9. The ¹H NMR spectrum of 3,4-(ditriethylene glycol) carboxaldehyde (**4**).

6. AmBH-PEG (5)

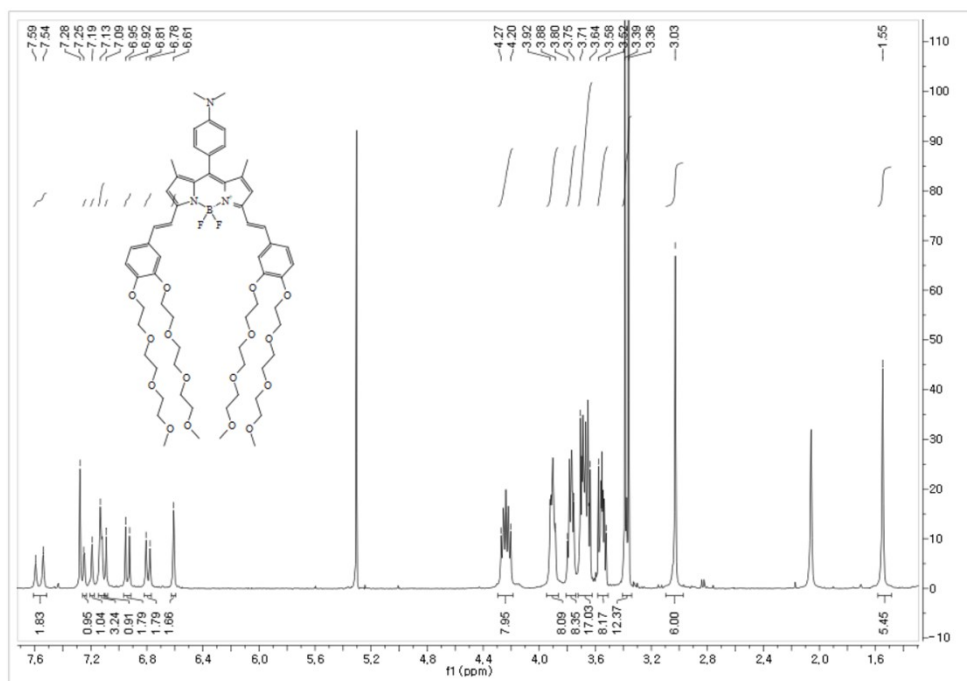


Figure S10. The ¹H NMR spectrum of AmBH-PEG (5).

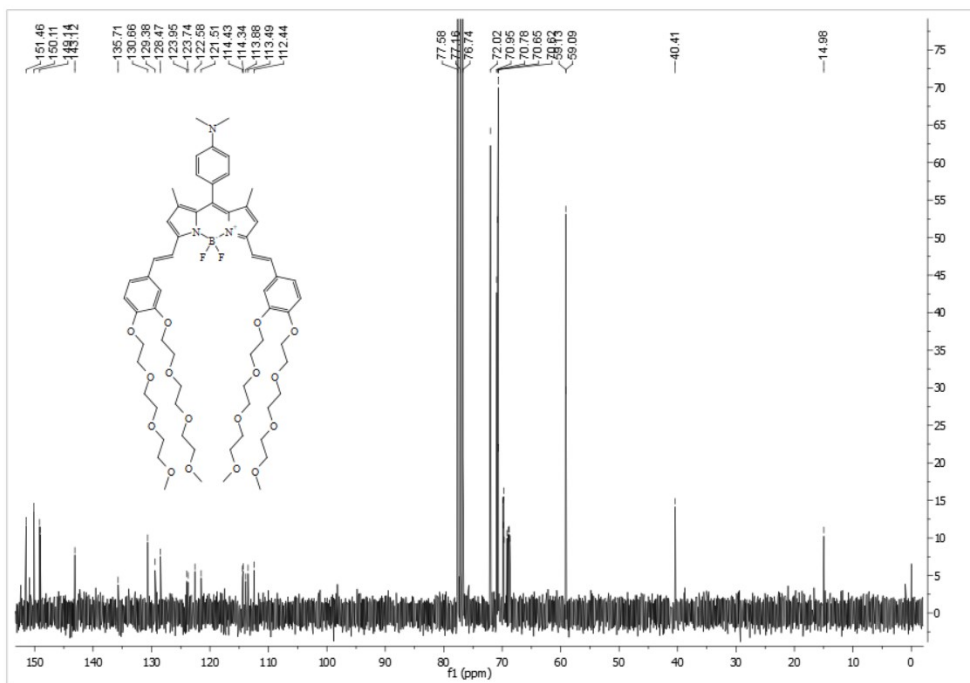


Figure S11. The ¹³C NMR spectrum of AmBH-PEG (5).

7. AmBM-PEG (6)

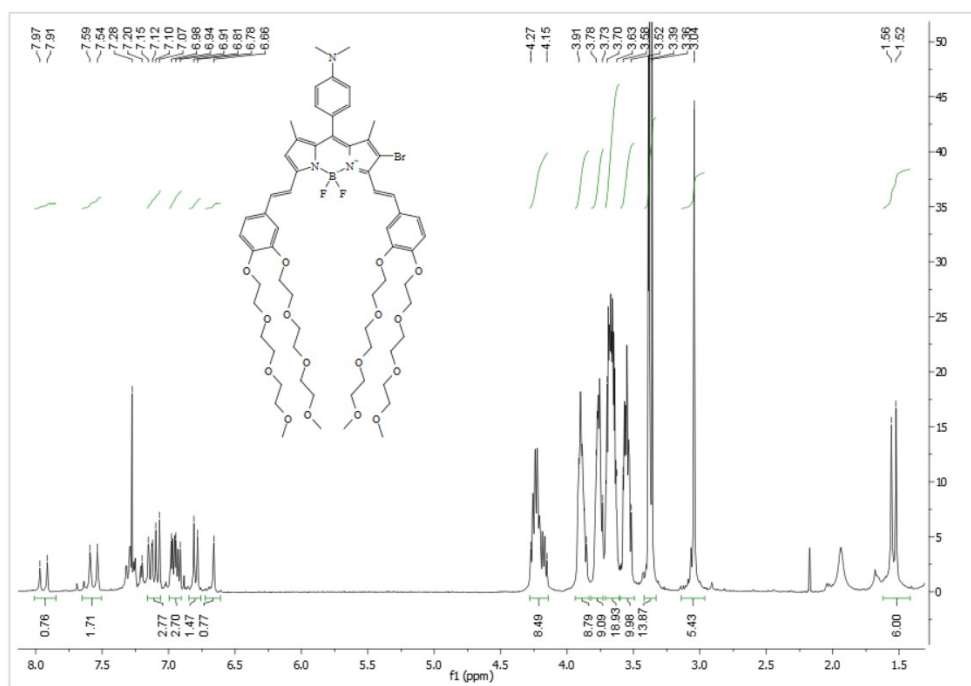


Figure S12. The ¹H NMR spectrum of AmBM-PEG (6).

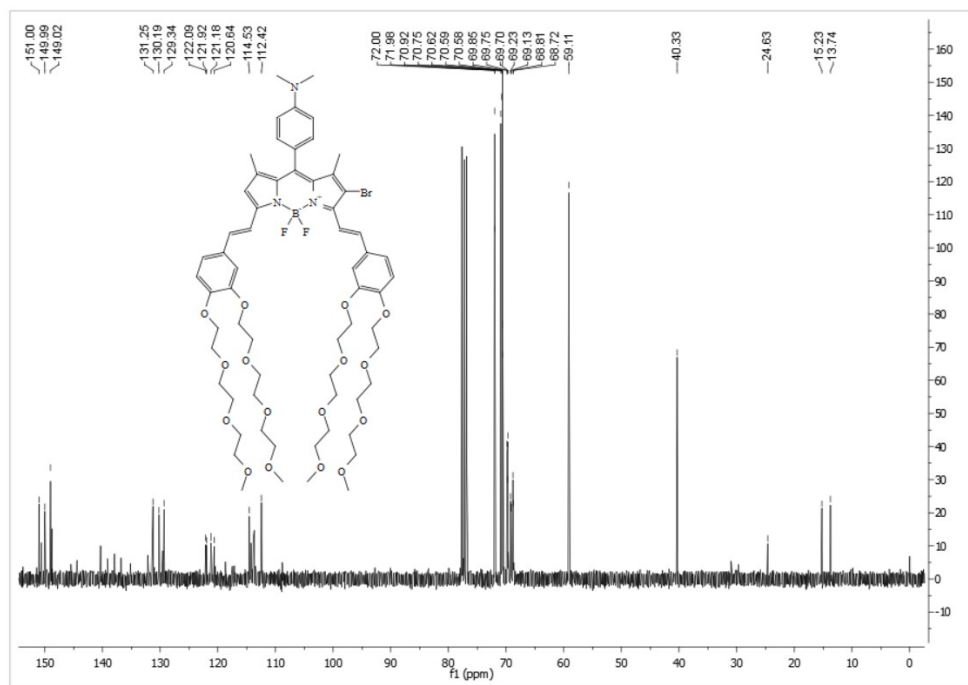


Figure S13. The ¹³C NMR spectrum of AmBM-PEG (6).

8. AmBBr-PEG (7)

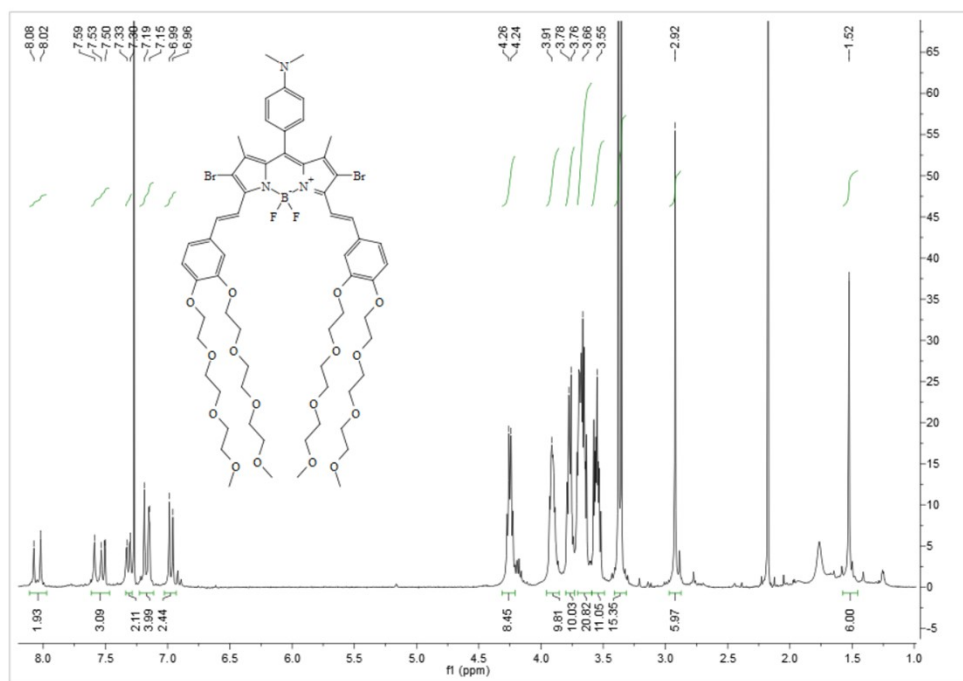


Figure S14. The ¹H NMR spectrum of AmBBr-PEG (7).

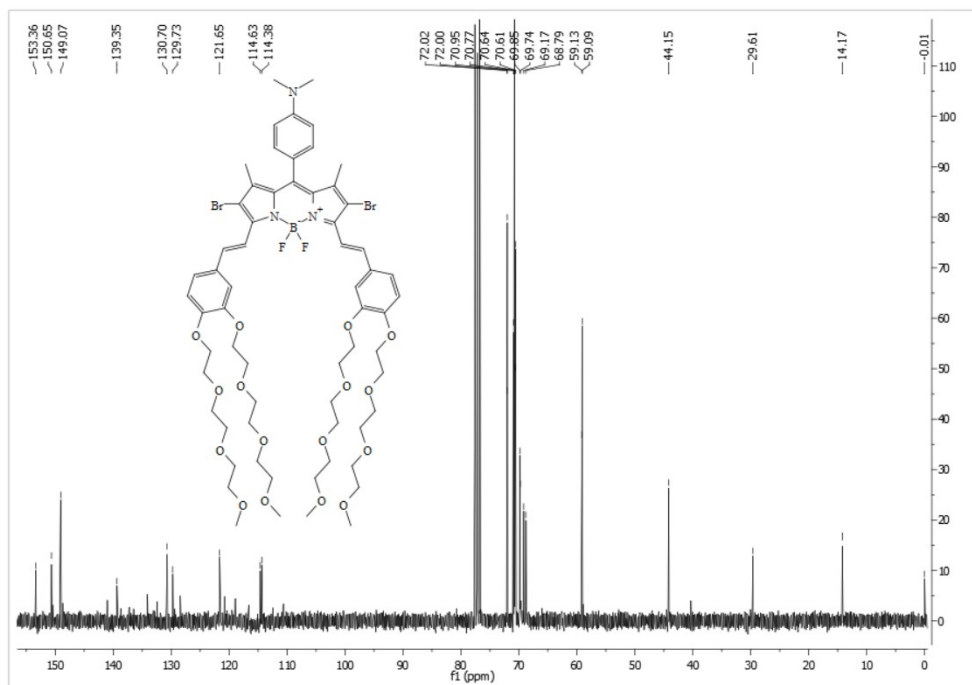


Figure S15. The ¹³C NMR spectrum of AmBBr-PEG (7).

9. AmBHI

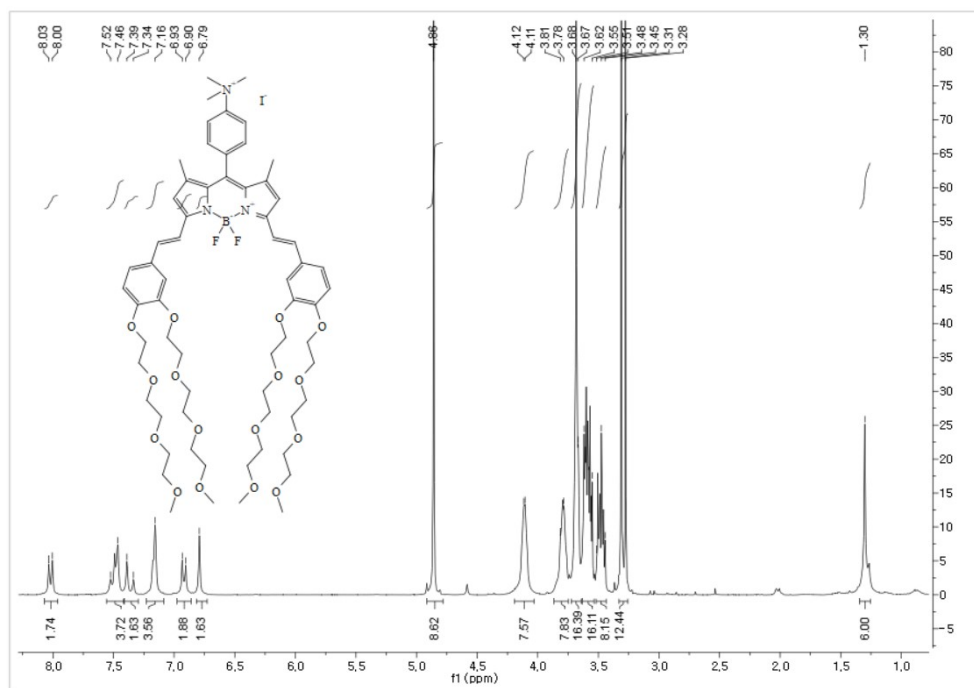


Figure S16. The ¹H NMR spectrum of AmBHI.

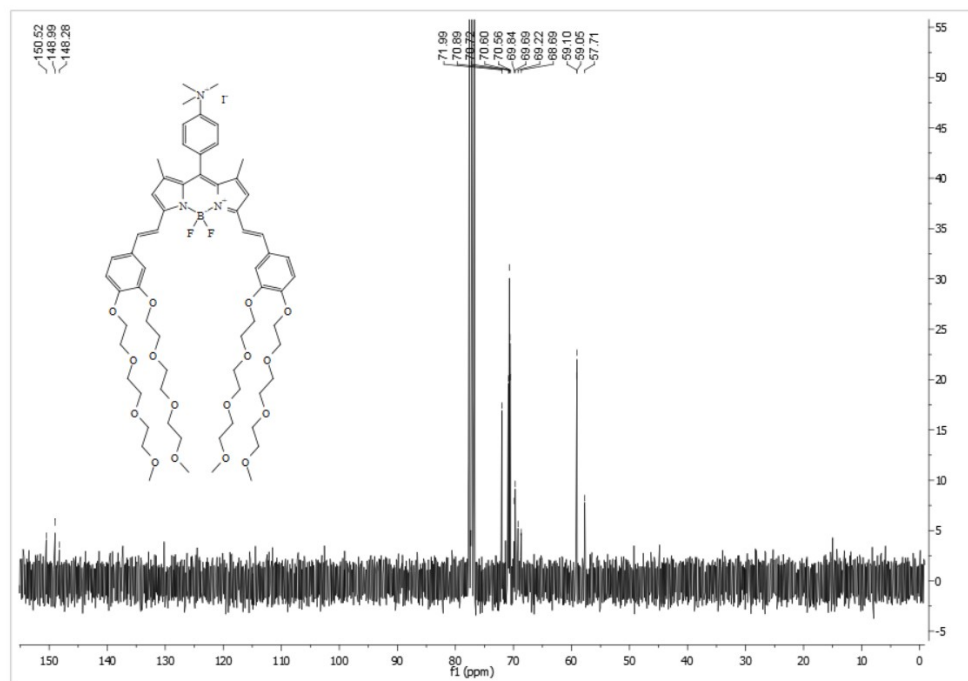


Figure S17. The ¹³C NMR spectrum of AmBHI.

10. AmBMI

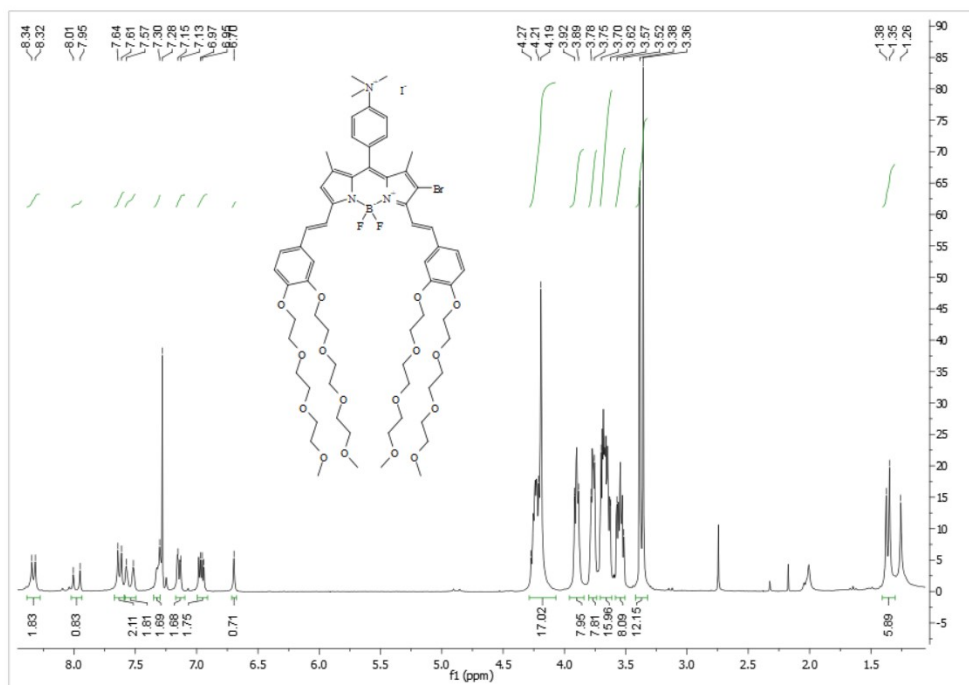


Figure S18. The ¹H NMR spectrum of AmBMI.

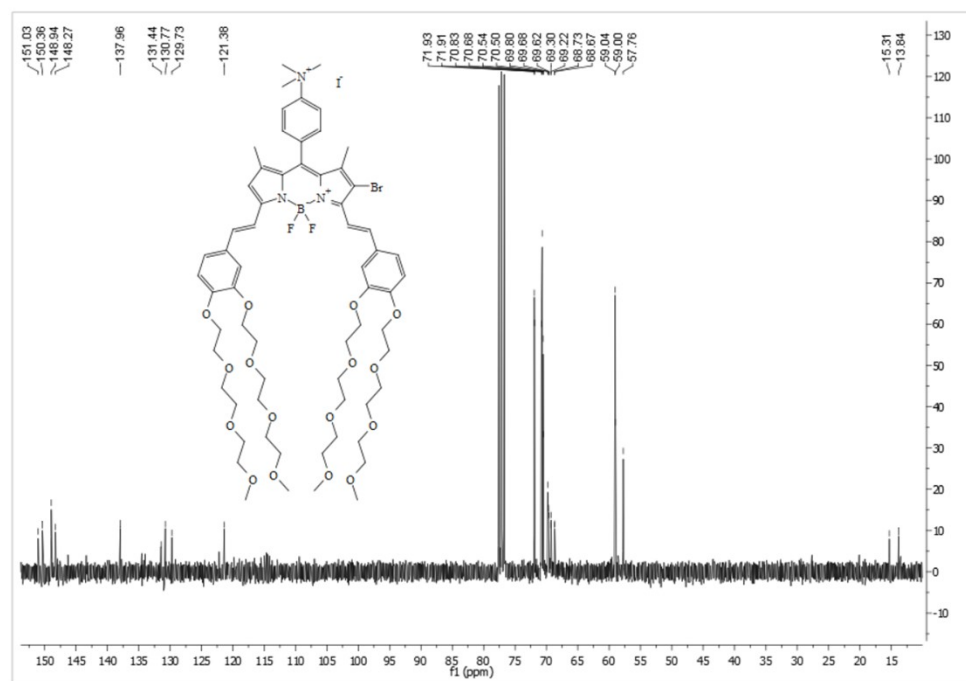


Figure S19. The ¹³C NMR spectrum of AmBMI.

11. AmBBrI

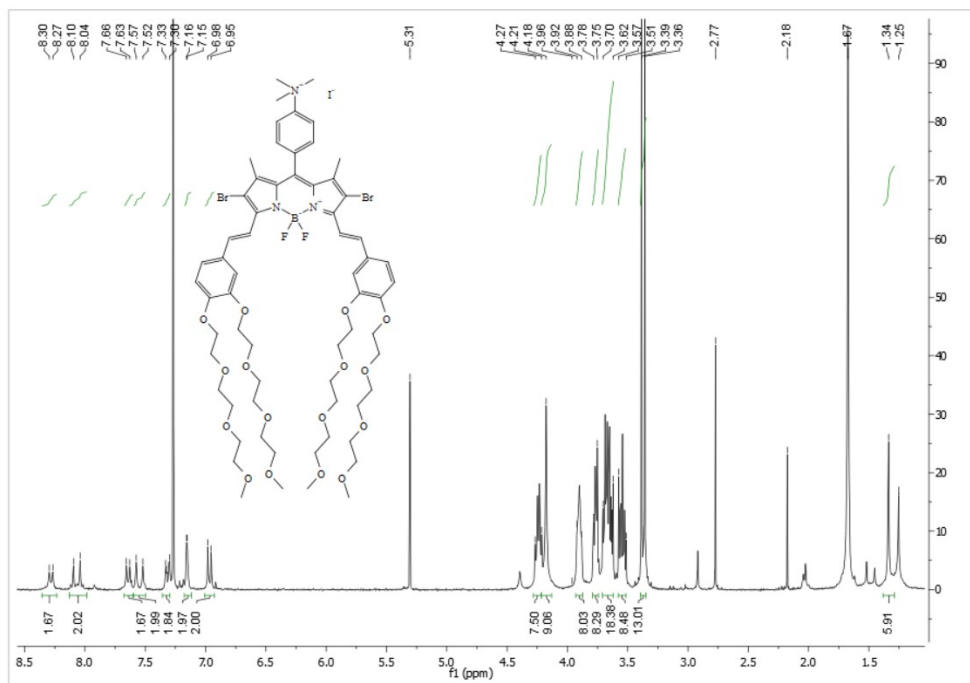


Figure S20. The ^1H NMR spectrum of AmBBrI.

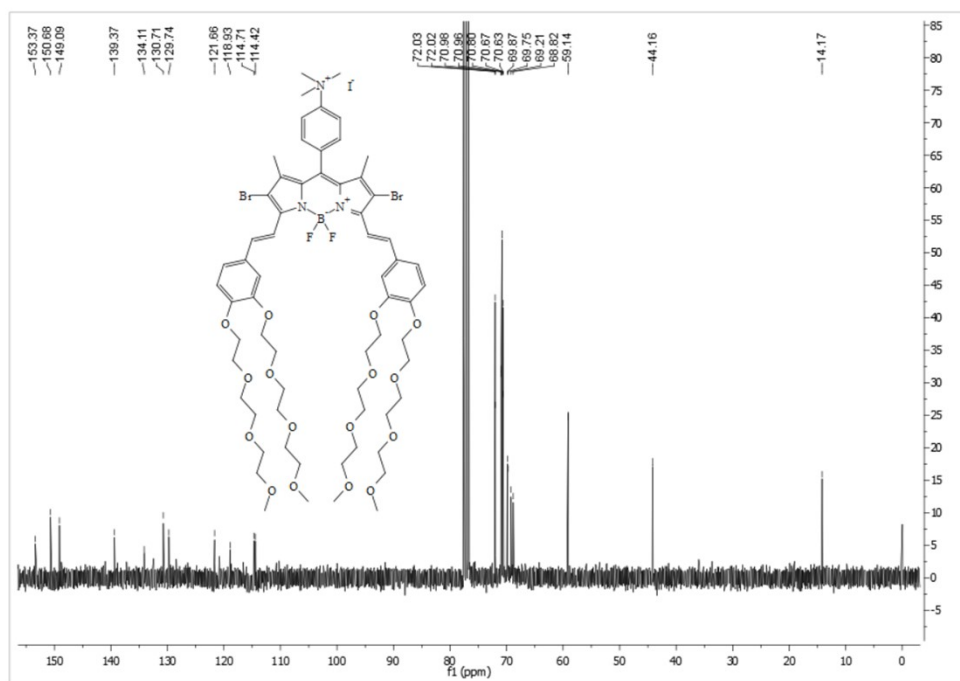


Figure S21. The ^{13}C NMR spectrum of AmBBrI.