

Supporting Information

Functionalization of BODIPY Dyes at 2,6-Positions through Formyl Groups

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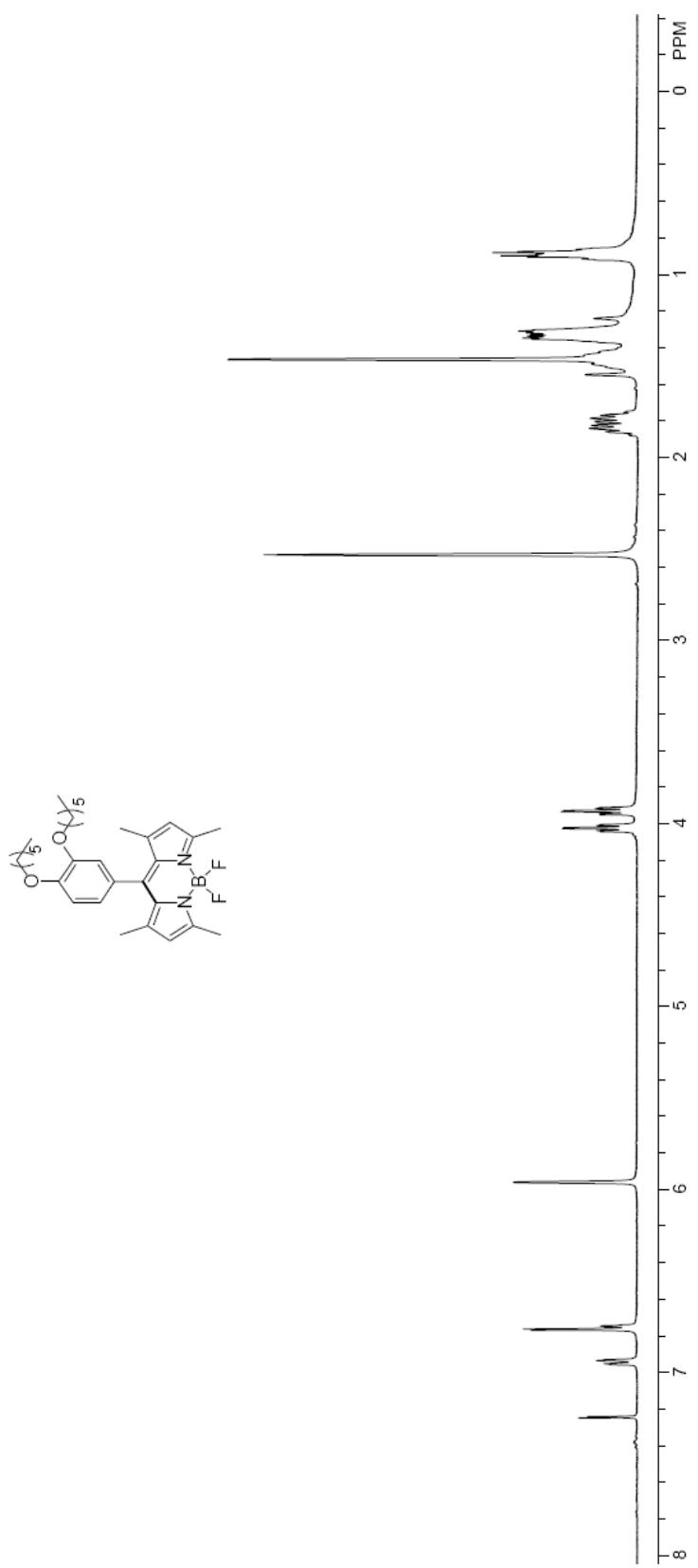


Figure S1. ^1H NMR spectrum of BODIPY dye 1 in CDCl_3 solution

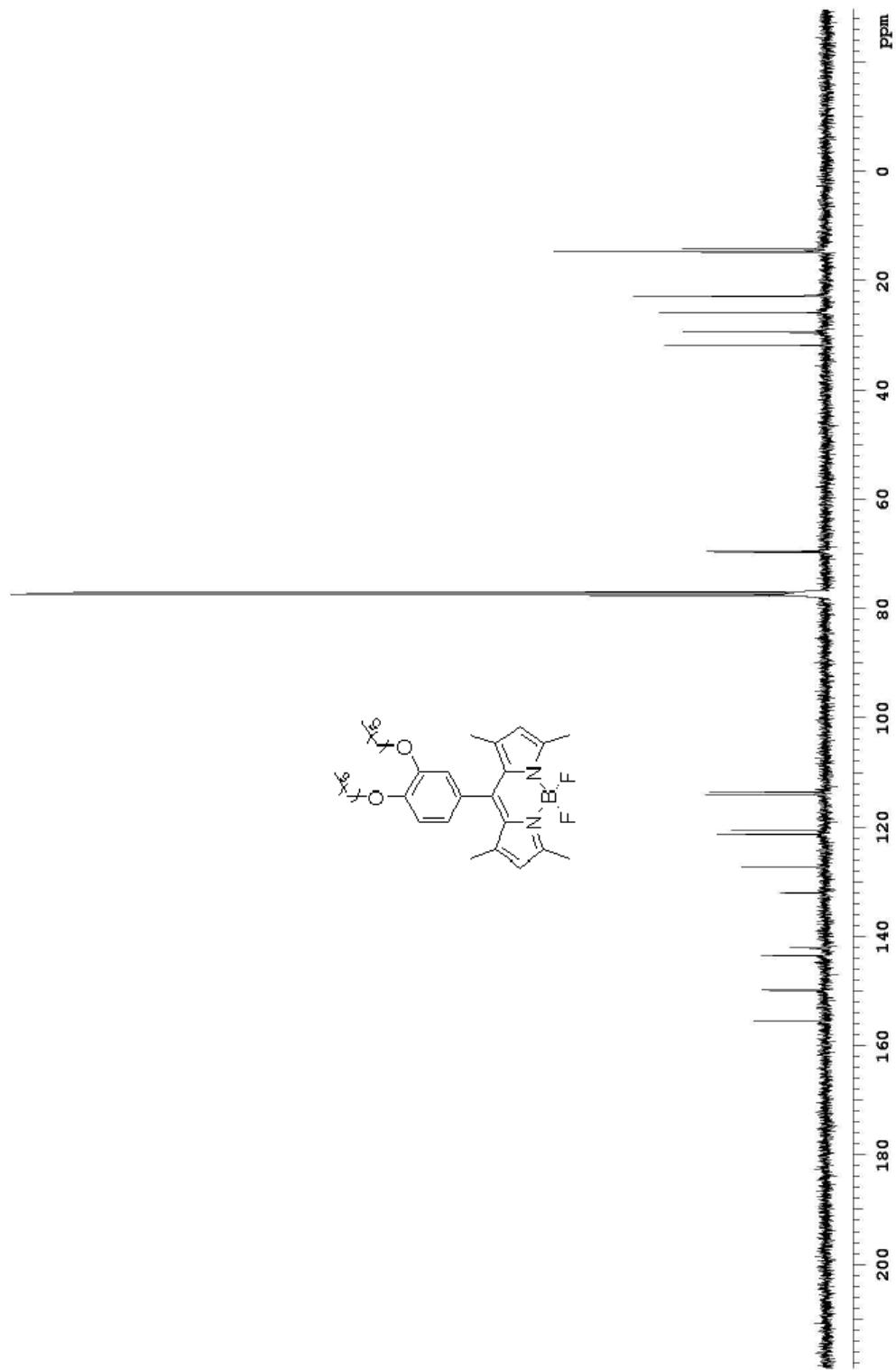


Figure S2. ^{13}C NMR spectrum of BODIPY dye 1 in CDCl_3 solution.

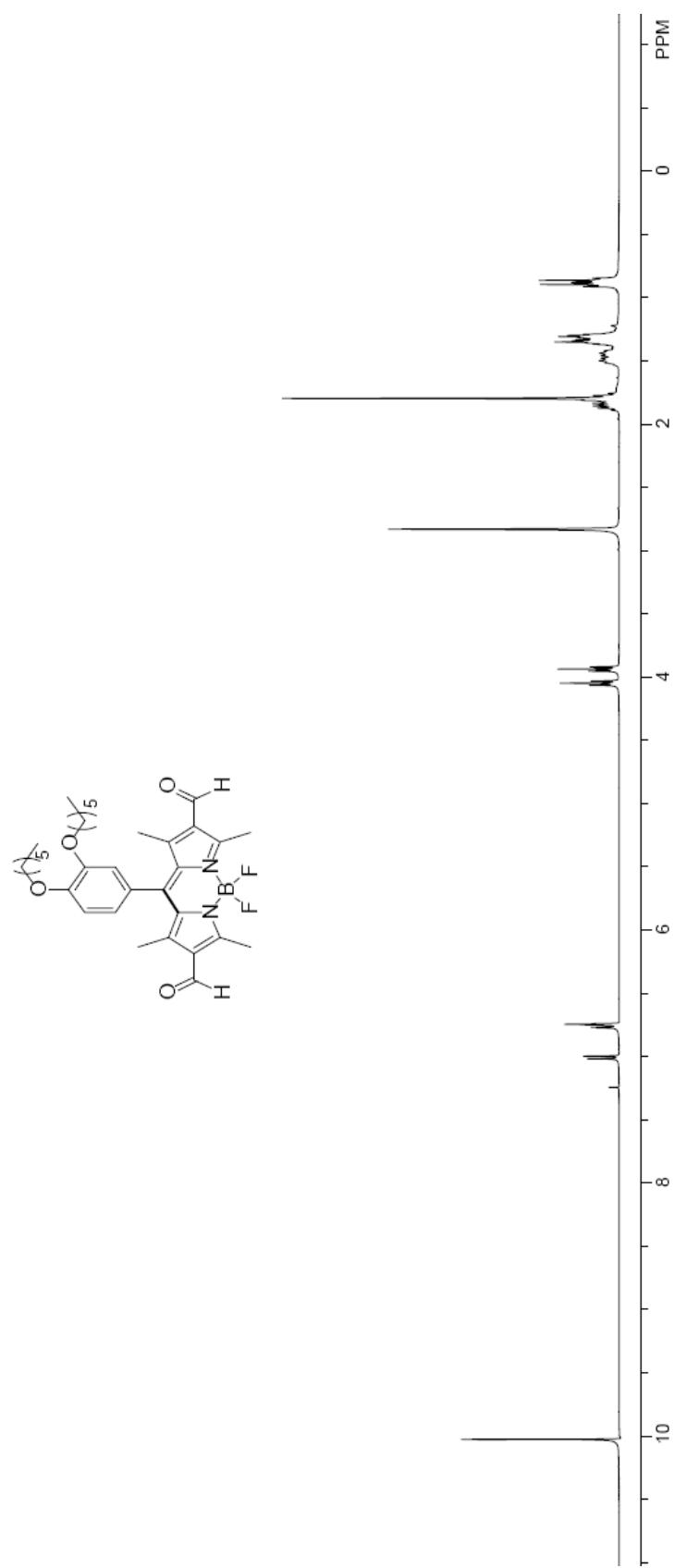


Figure S3. ^1H NMR spectrum of BODIPY dye **3** in CDCl_3 solution.

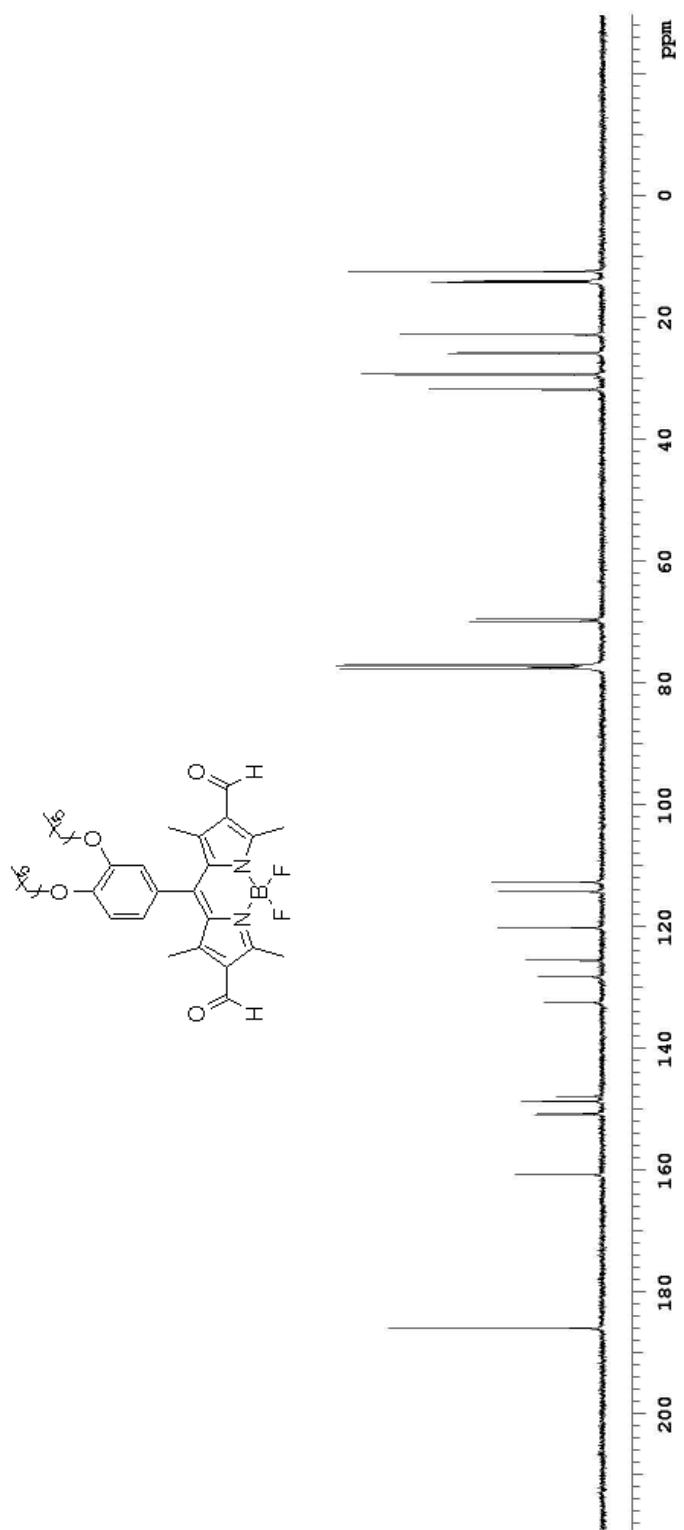


Figure S4. ^{13}C NMR spectrum of BODIPY dye 3 in CDCl_3 solution.

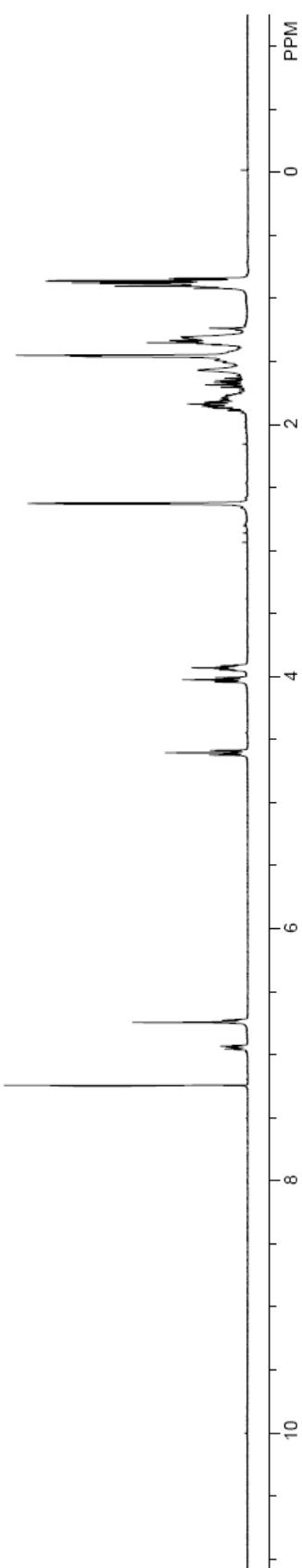
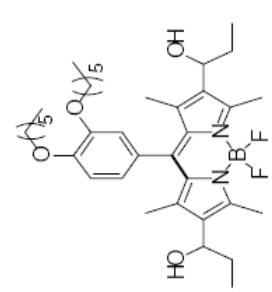


Figure S5. ^1H NMR spectrum of BODIPY dye 4 in CDCl_3 solution.

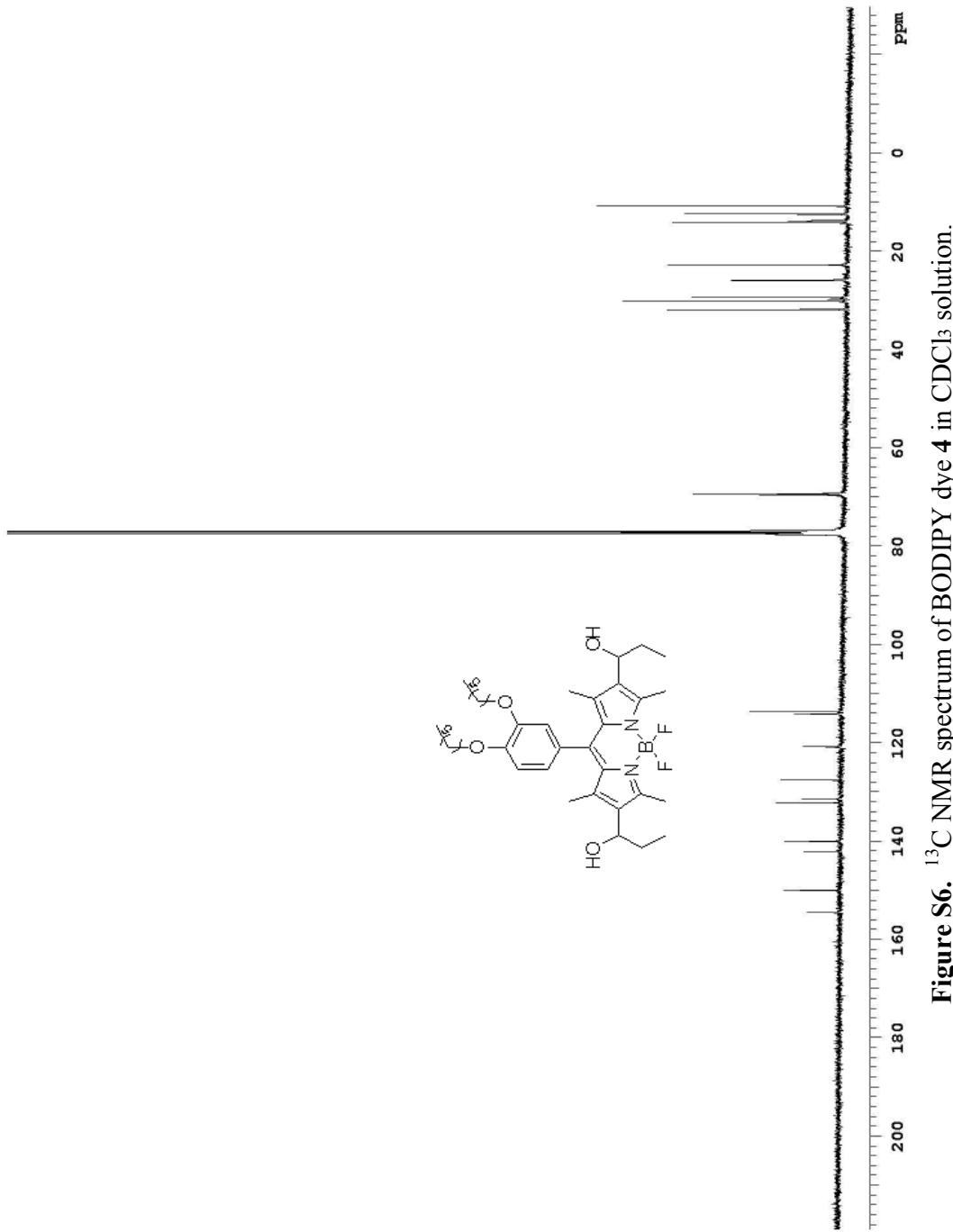


Figure S6. ^{13}C NMR spectrum of BODIPY dye 4 in CDCl_3 solution.

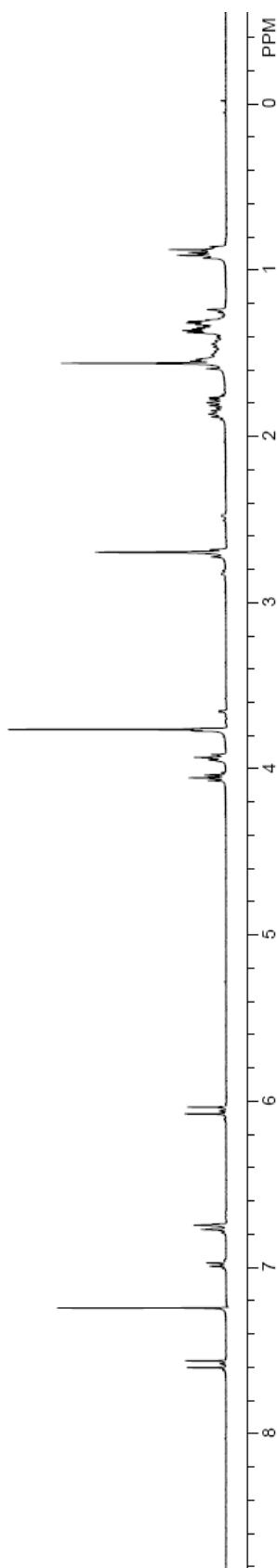
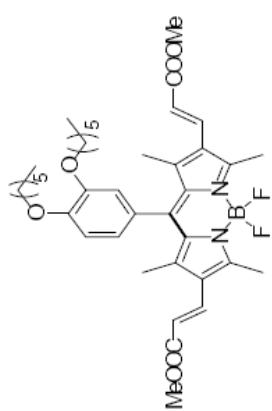


Figure S7. ^1H NMR spectrum of BODIPY dye 5 in CDCl_3 solution.

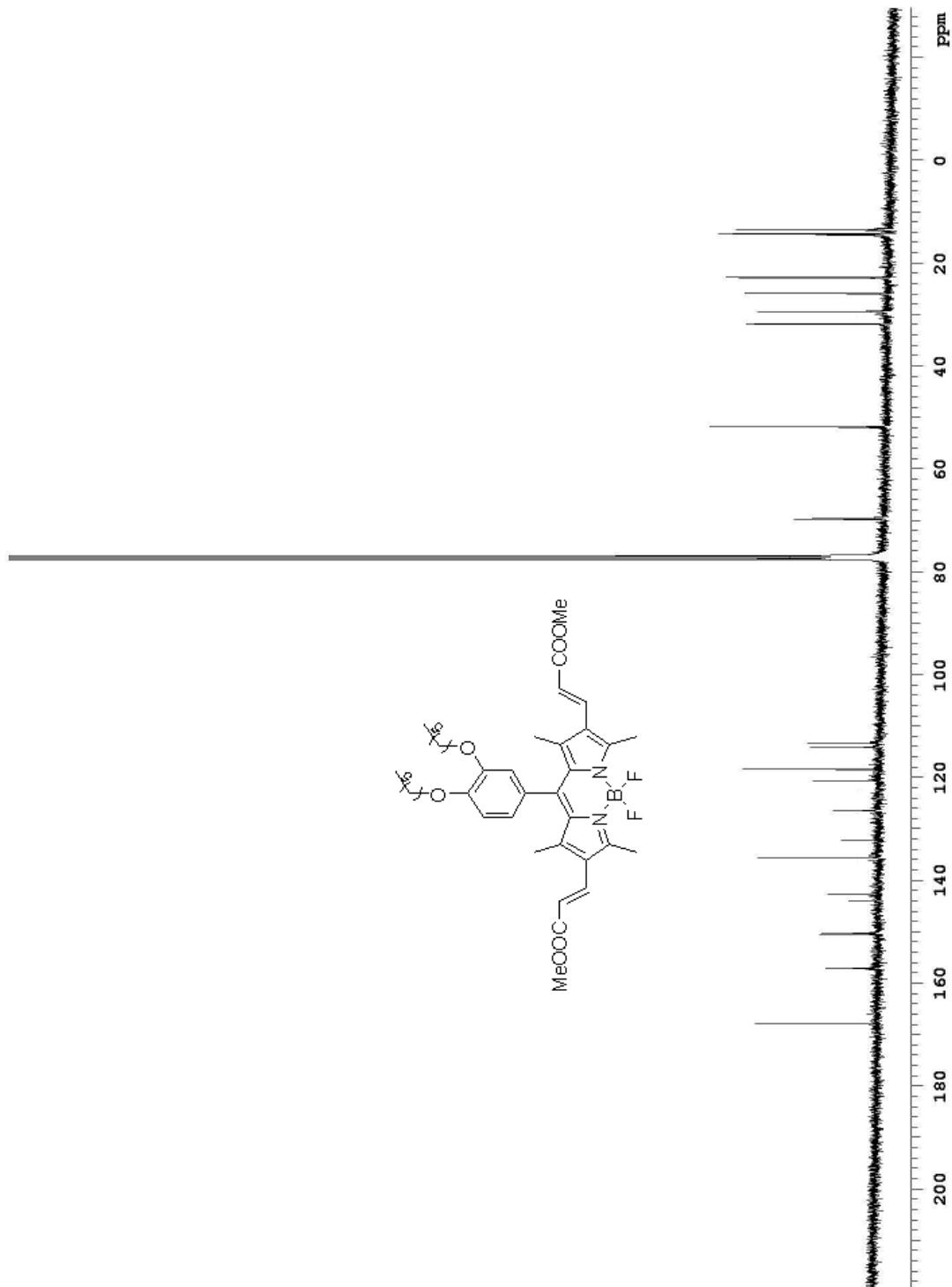


Figure S8. ^{13}C NMR spectrum of BODIPY dye **5** in CDCl_3 solution.

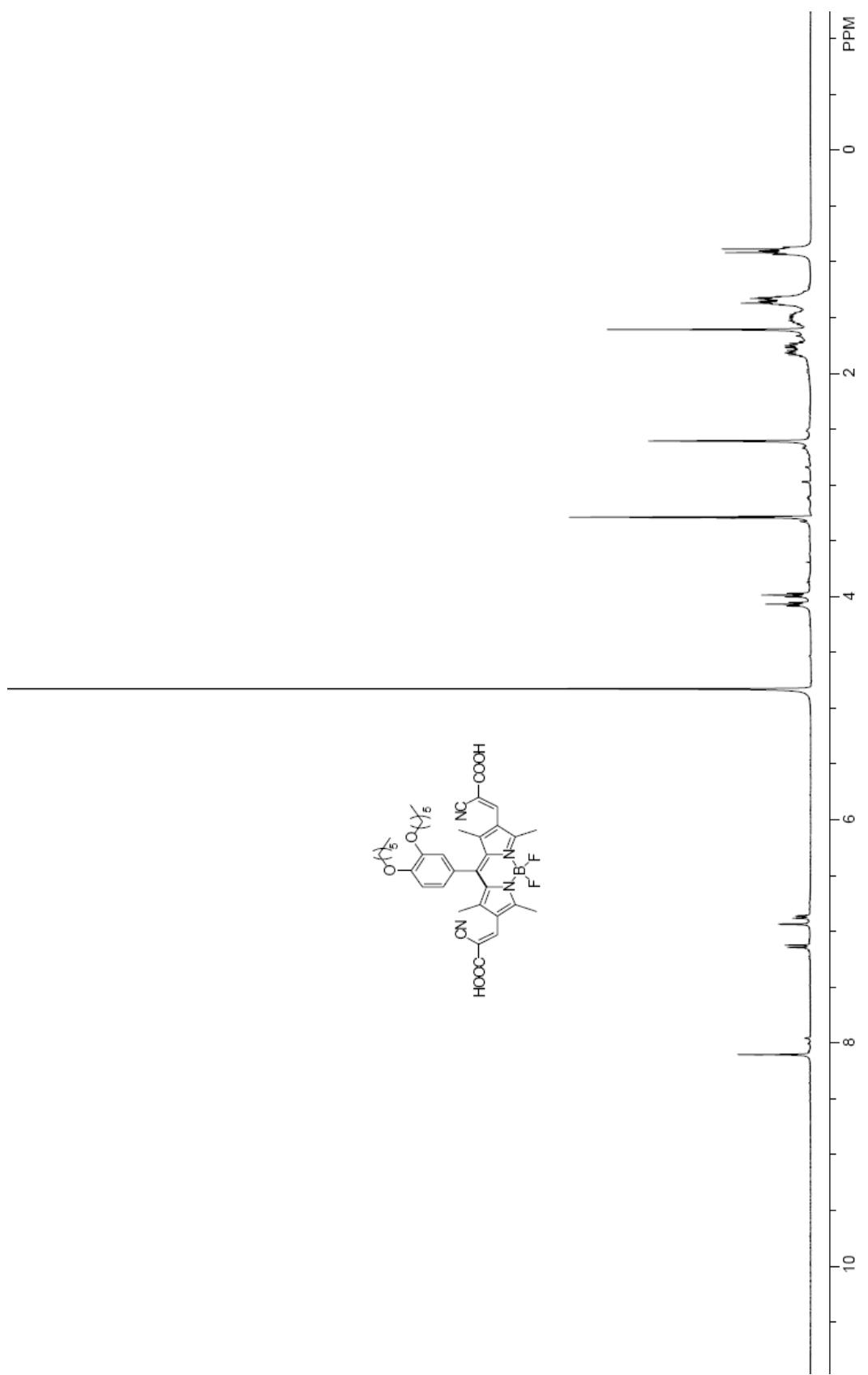


Figure S9. ^1H NMR spectrum of BODIPY dye 6 in CD_3OD solution.

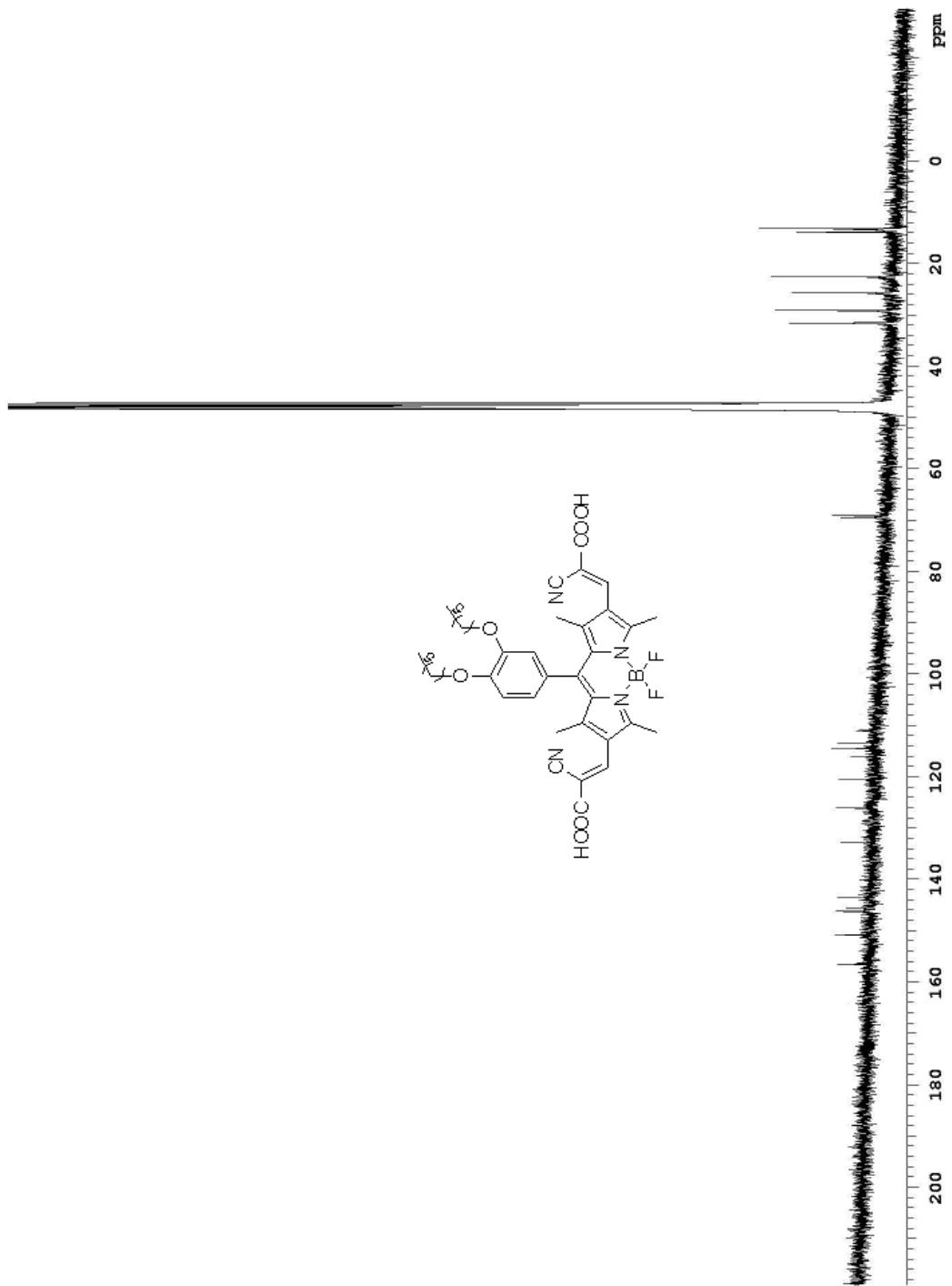


Figure S10. ^{13}C NMR spectrum of BODIPY dye 6 in CD_3OD solution.

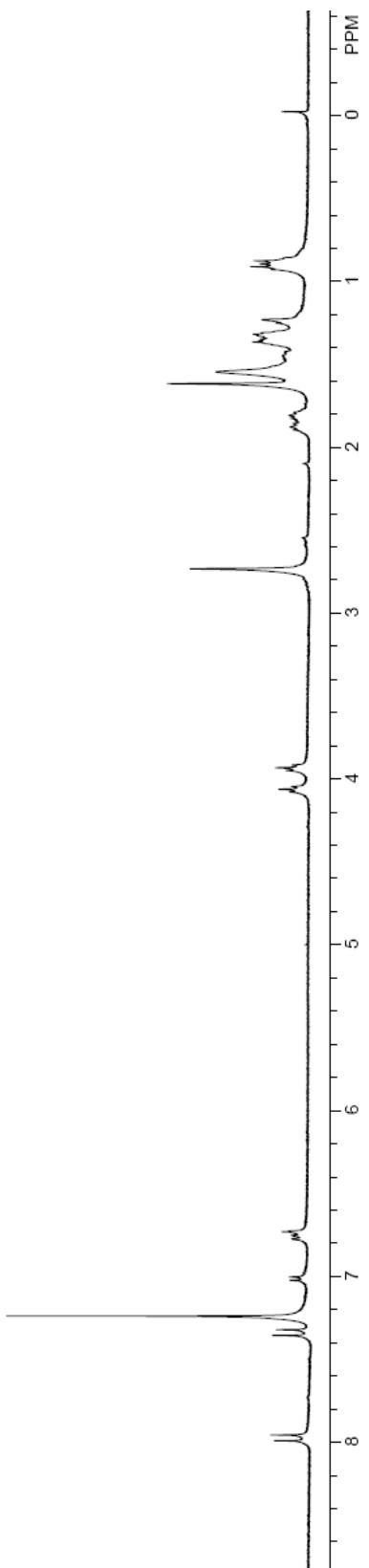
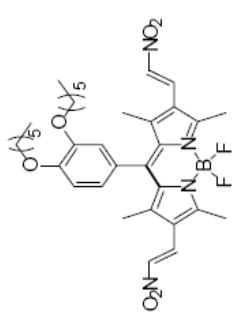


Figure S11. ^1H NMR spectrum of BODIPY dye **7a** in CDCl_3 solution.

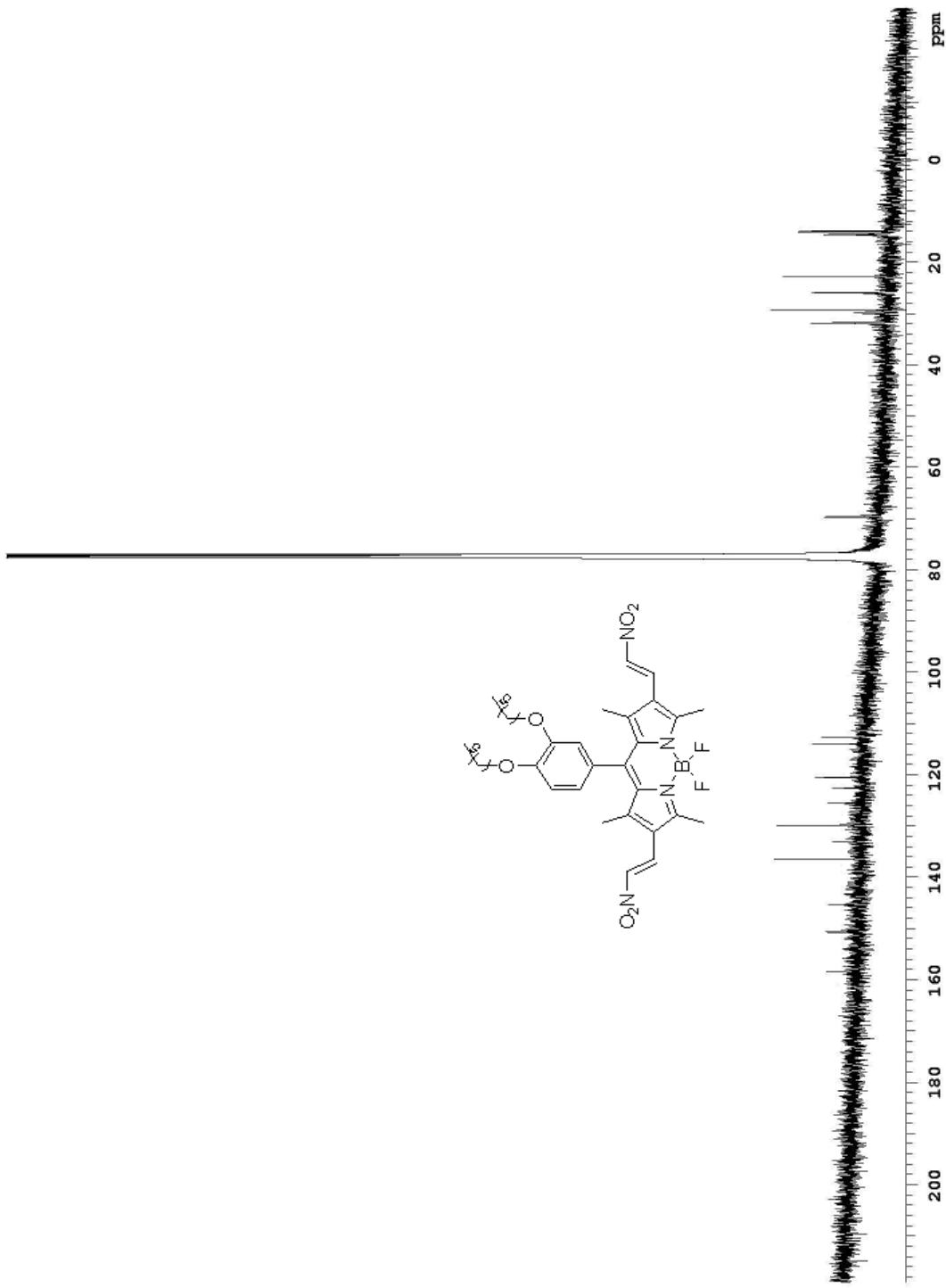


Figure S12. ^{13}C NMR spectrum of BODIPY dye 7a in CDCl_3 solution.

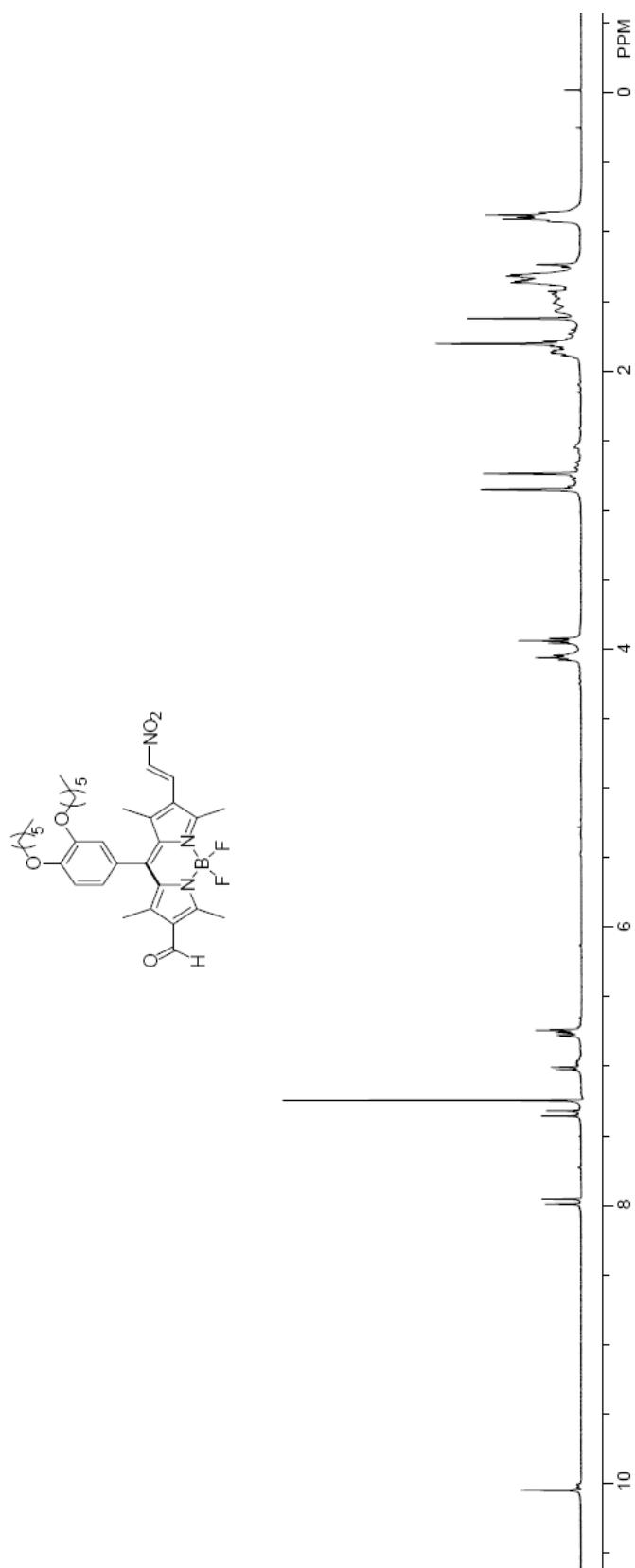


Figure S13. ¹H NMR spectrum of BODIPY dye **7b** in CDCl₃ solution.

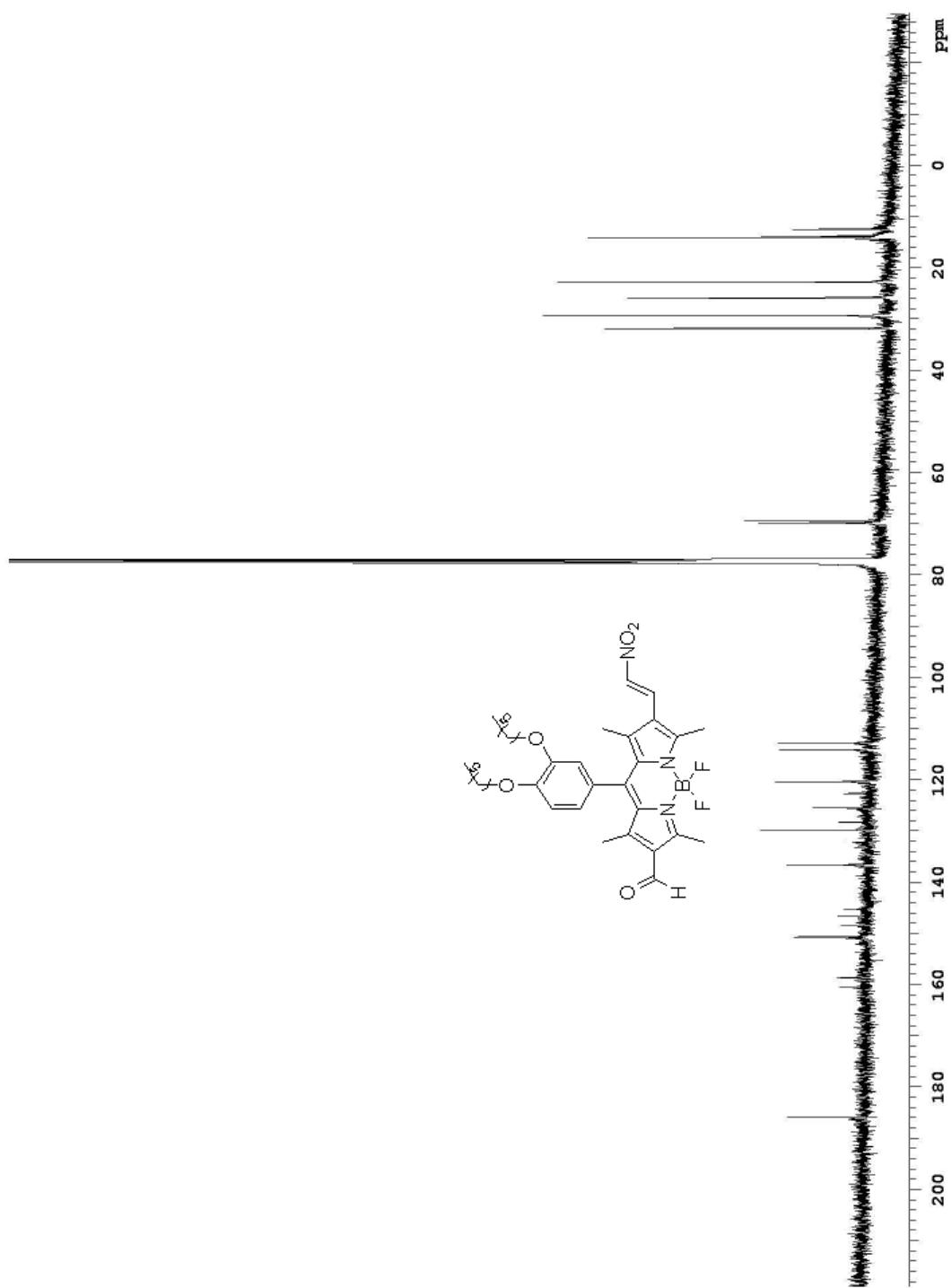


Figure S14. ^{13}C NMR spectrum of BODIPY dye **7b** in CDCl_3 solution.

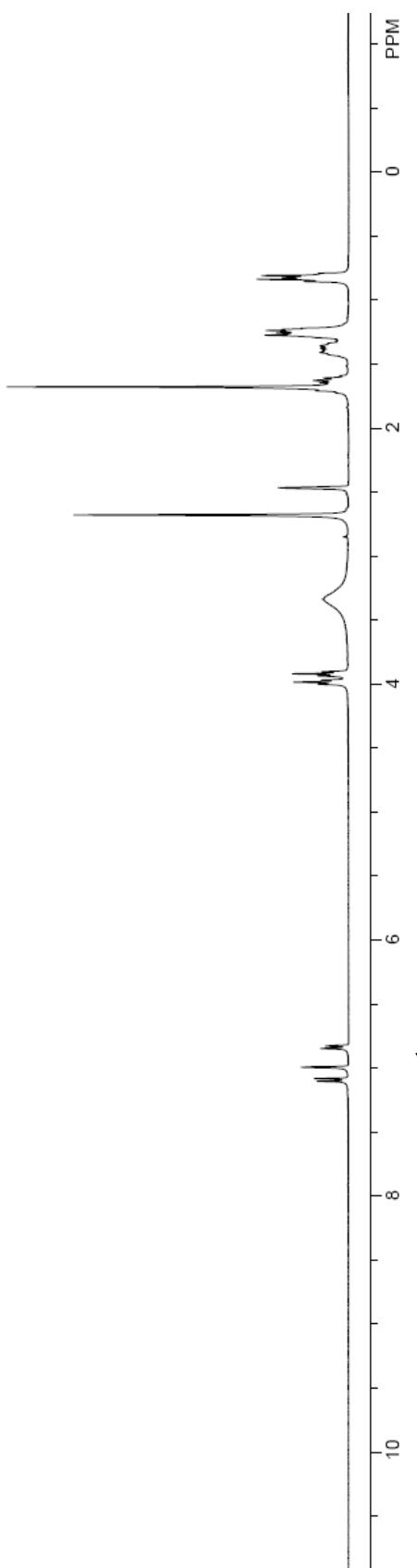
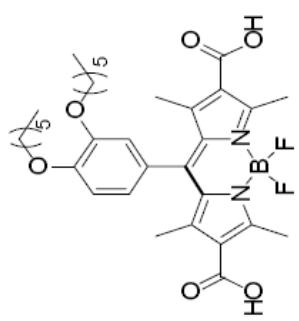


Figure S15. ^1H NMR spectrum of BODIPY dye 8 in DMSO-d₆ solution.

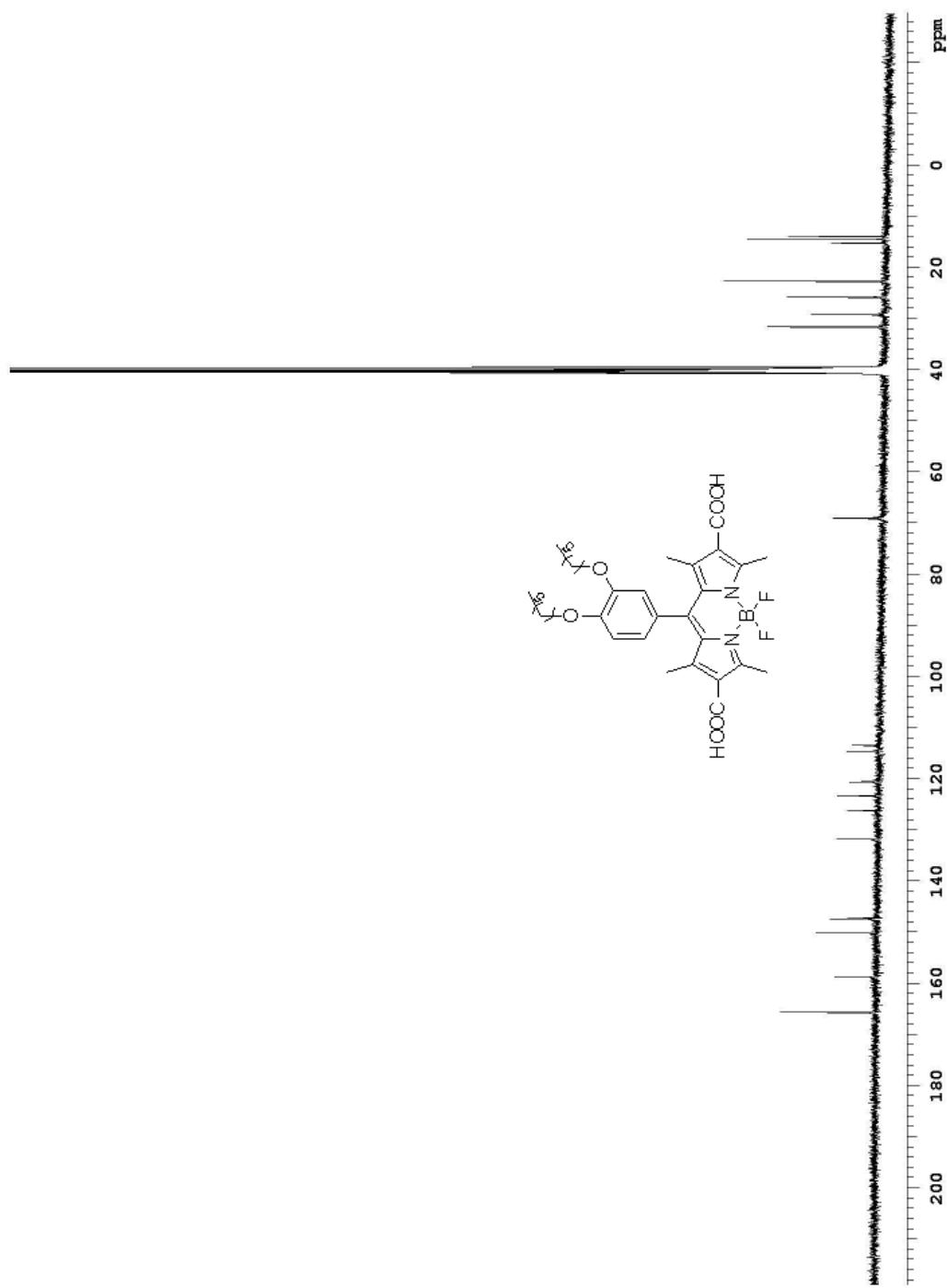


Figure S16. ^{13}C NMR spectrum of BODIPY dye **8** in DMSO-d_6 solution.

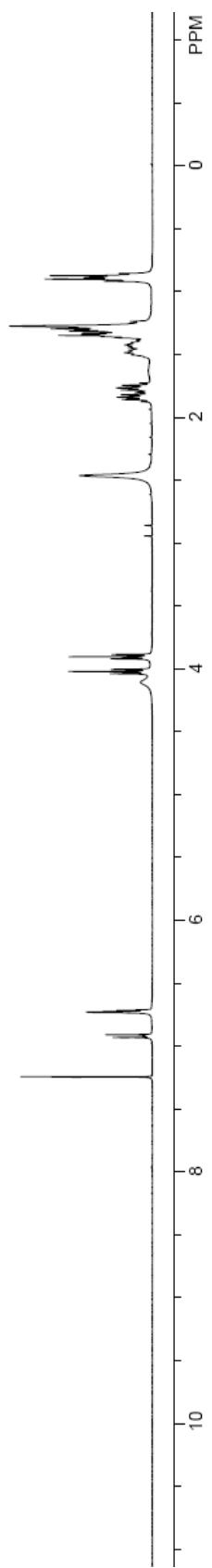
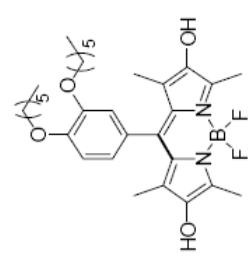


Figure S17. ^1H NMR spectrum of BODIPY dye 10 in CDCl_3 solution.

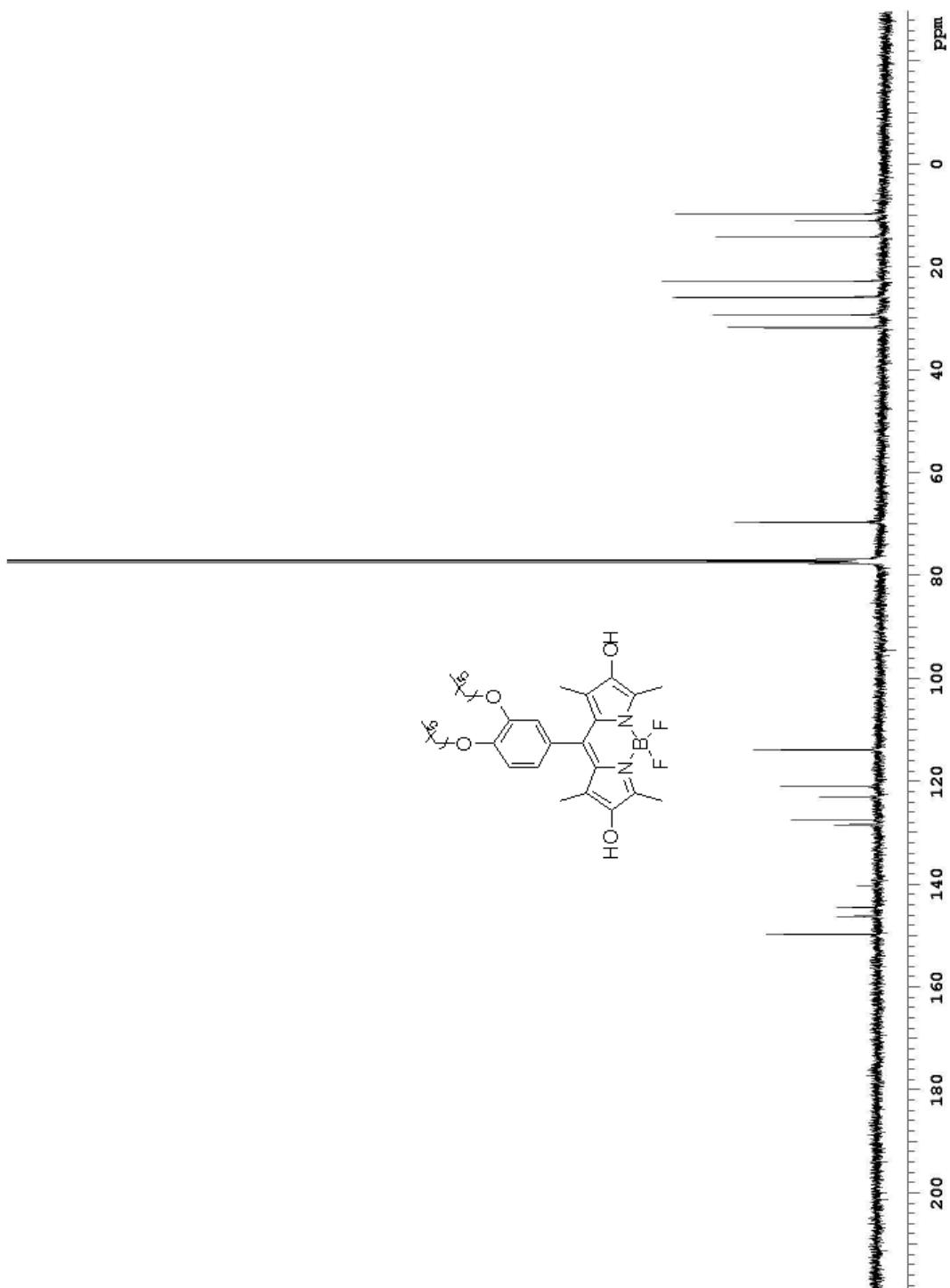


Figure S18. ^{13}C NMR spectrum of BODIPY dye 10 in CDCl_3 solution.

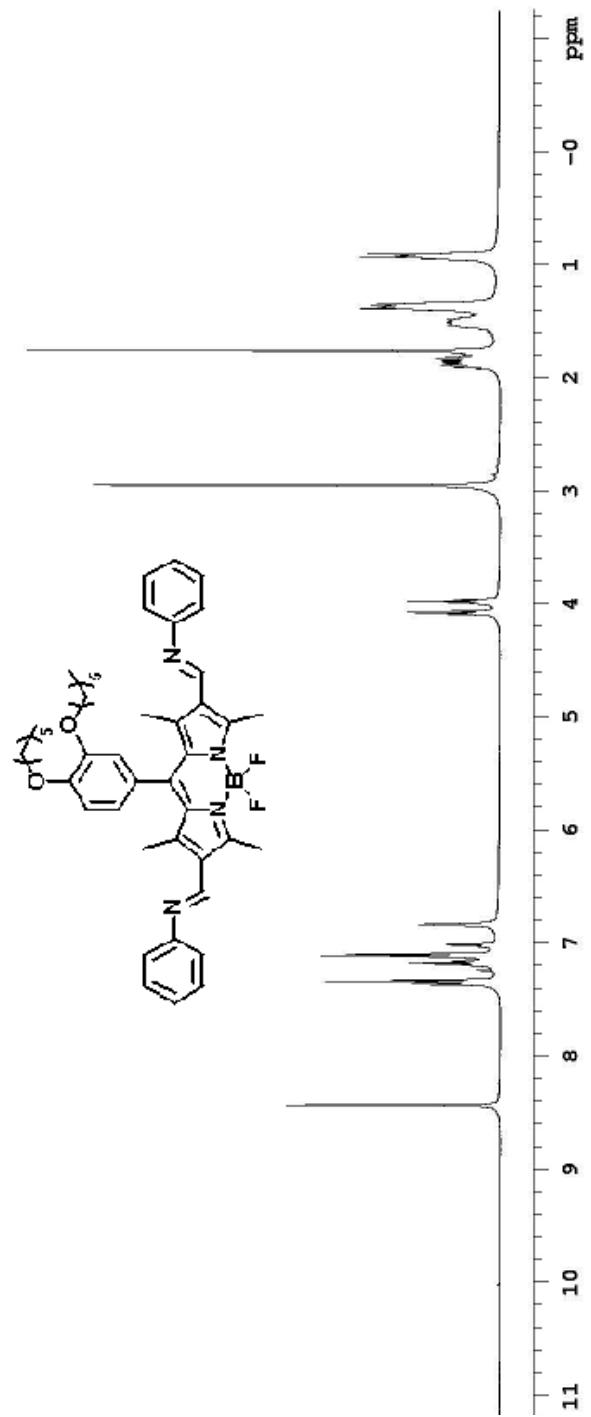


Figure S19. ¹H NMR spectrum of BODIPY dye 11 in CDCl₃ solution.

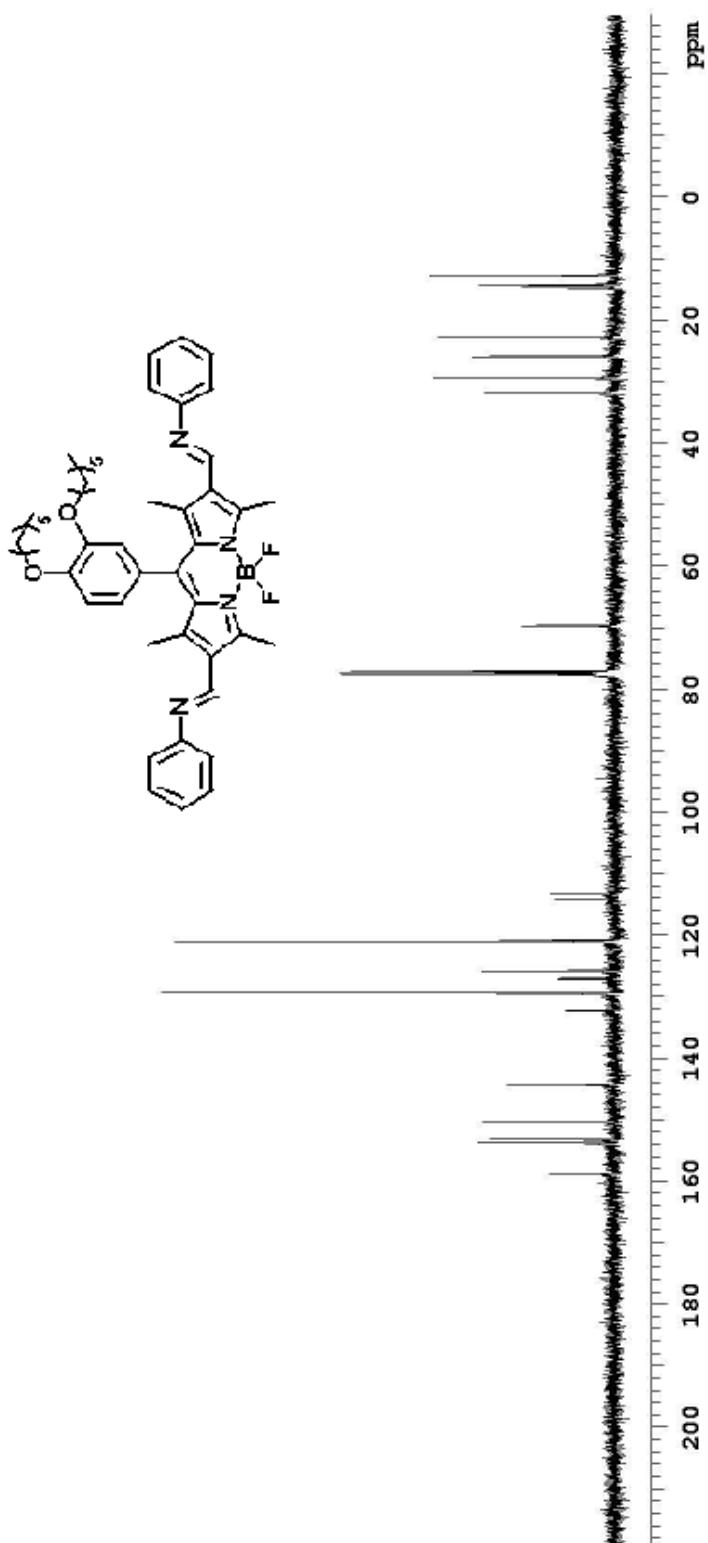


Figure S20. ^{13}C NMR spectrum of BODIPY dye 11 in CDCl_3 solution.

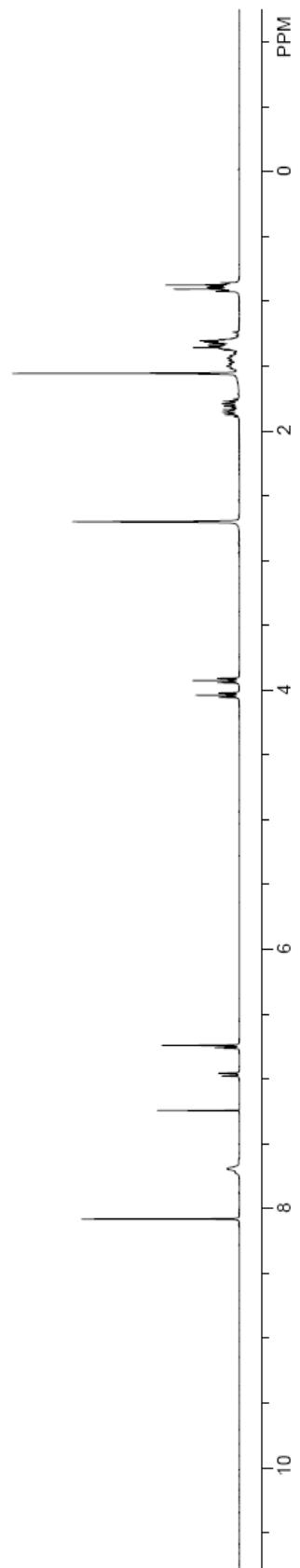
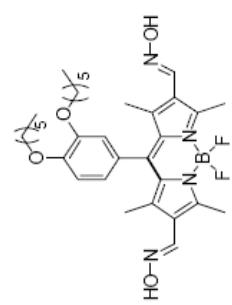


Figure S21. ^1H NMR spectrum of BODIPY dye 12 in CDCl_3 solution.

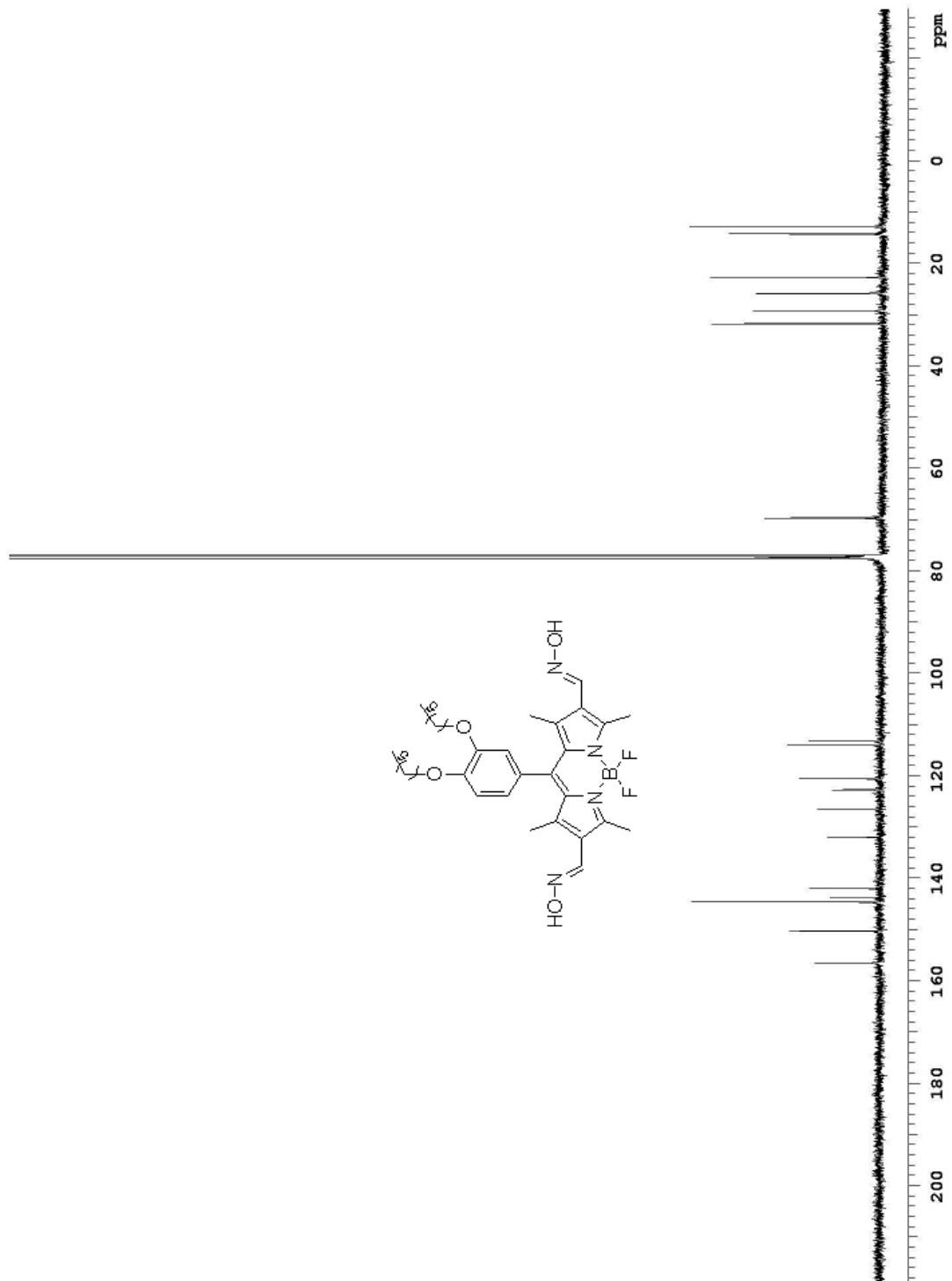


Figure S22. ^{13}C NMR spectrum of BODIPY dye 12 in CDCl_3 solution.

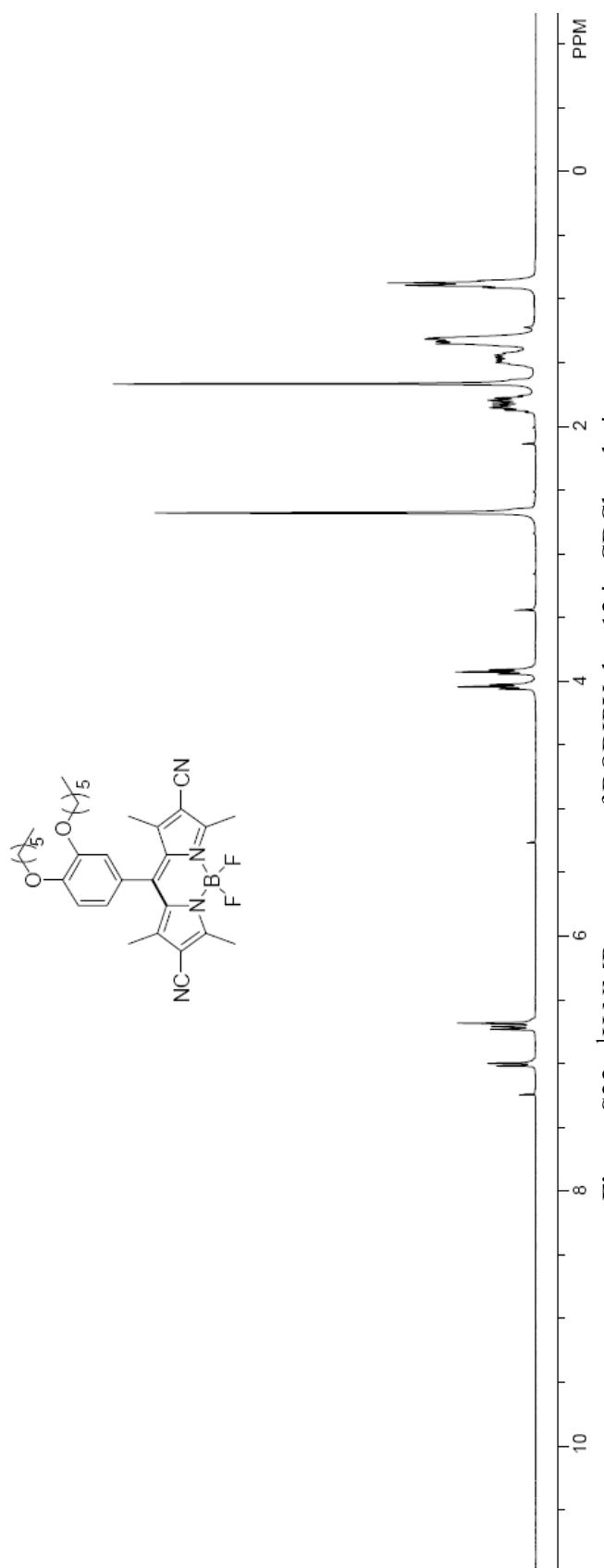


Figure S23. ^1H NMR spectrum of BODIPY dye 13 in CDCl_3 solution.

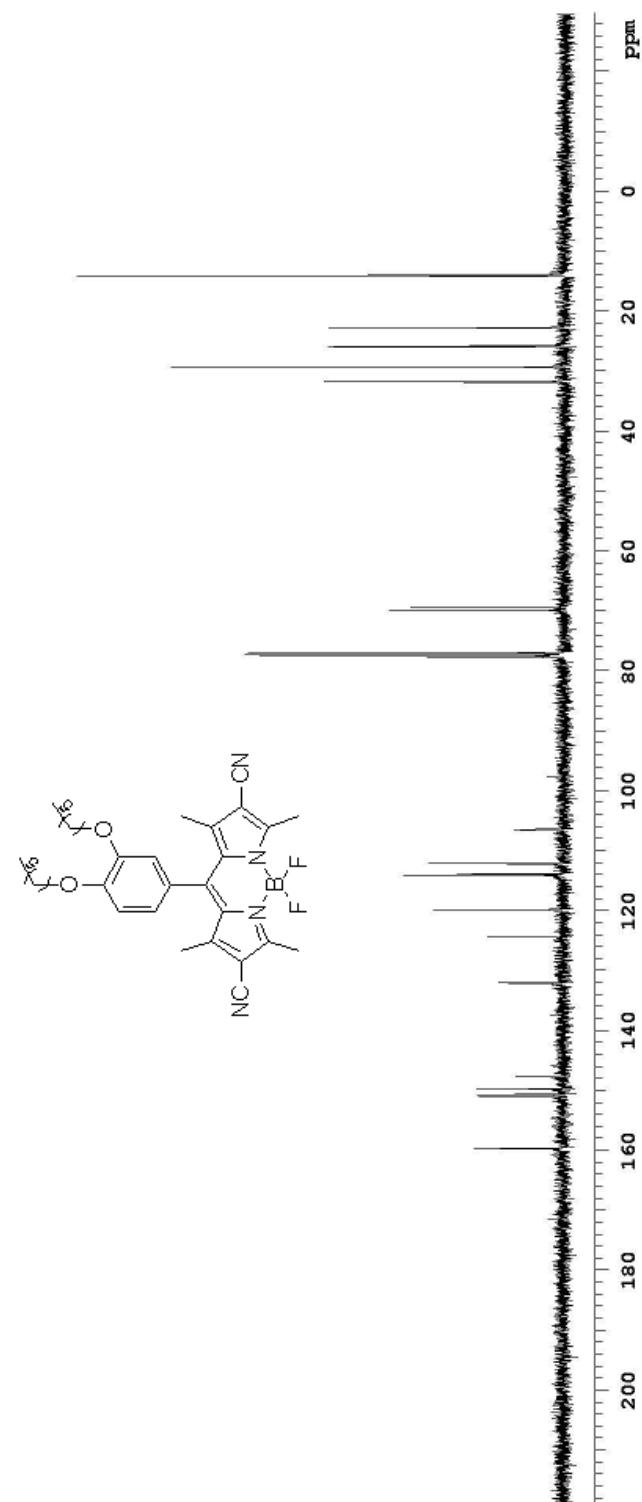


Figure S24. ^{13}C NMR spectrum of BODIPY dye 13 in CDCl_3 solution

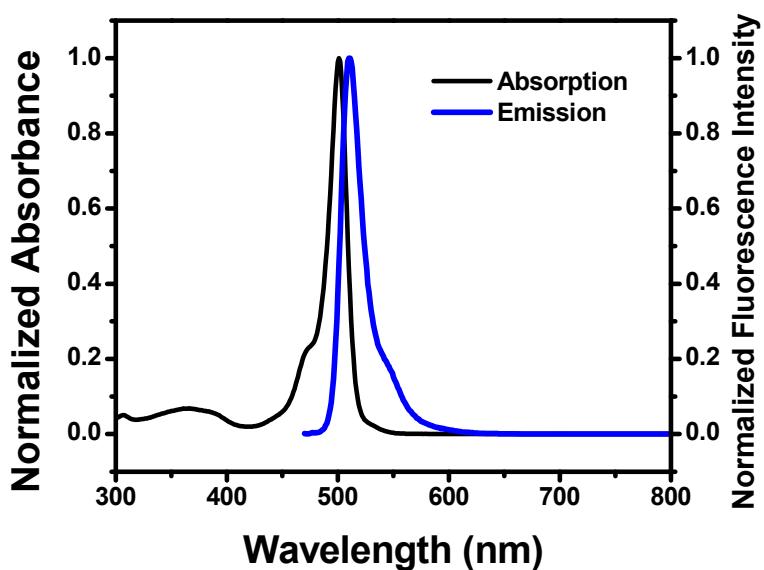


Figure S25. Absorption and Emission spectra of BODIPY dye **1** in dichloromethane solution (excitation wavelength = 460 nm).

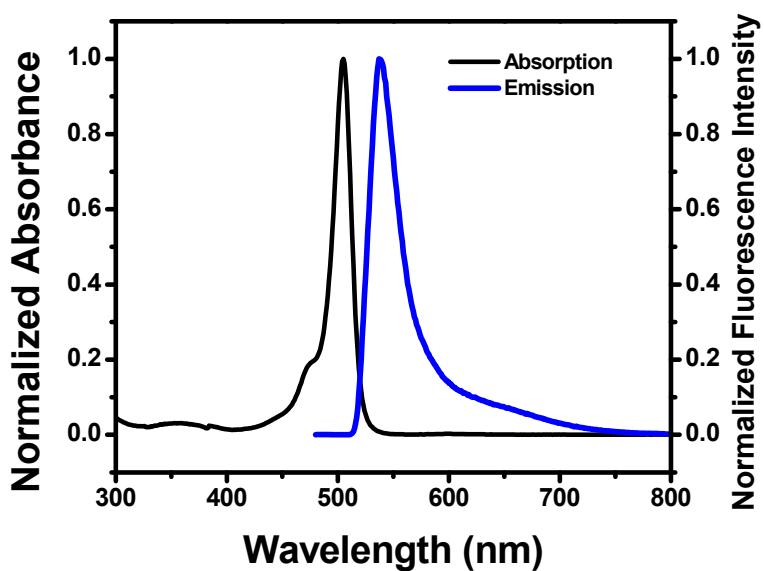


Figure S26. Absorption and Emission spectra of BODIPY dye **3** in dichloromethane solution (excitation wavelength = 470 nm).

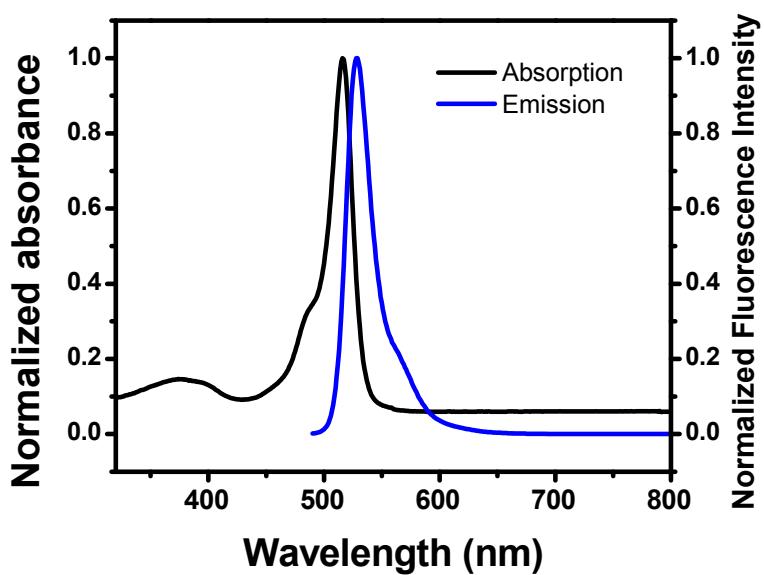


Figure S27. Absorption and Emission spectra of BODIPY dye 4 in dichloromethane (excitation wavelength = 480 nm).

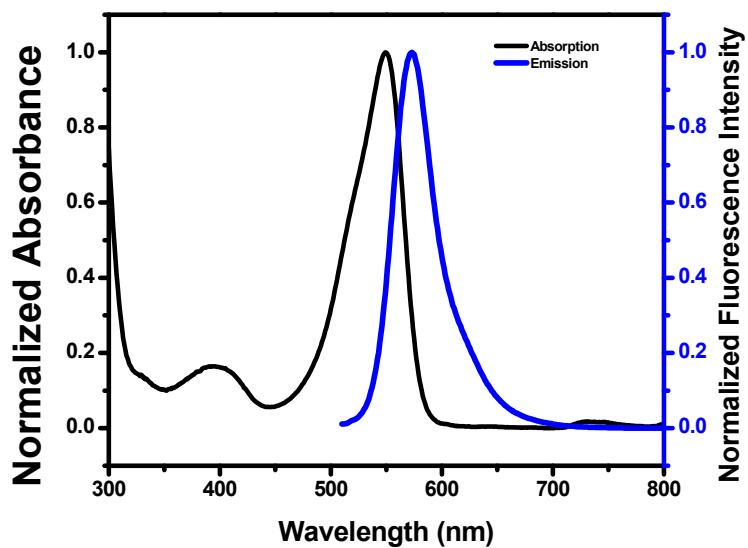


Figure S28. Absorption and Emission spectra of BODIPY dye 5 in dimethyl sulfoxide (excitation wavelength = 500 nm).

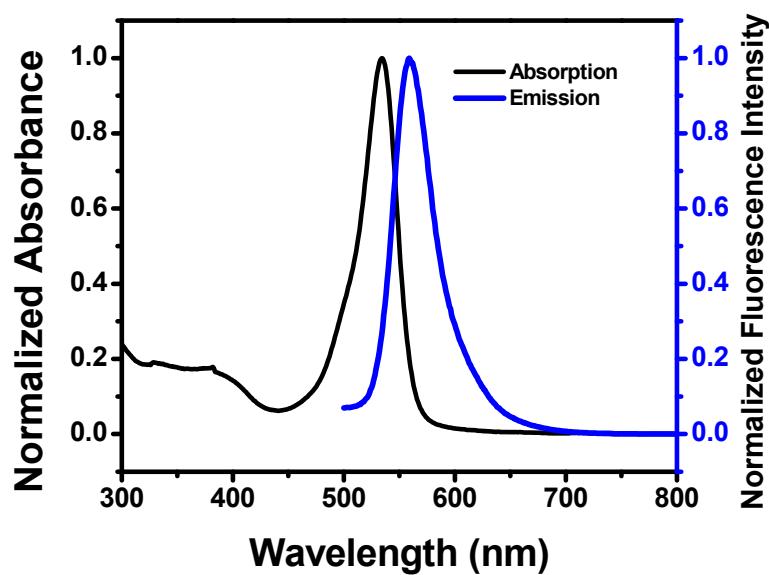


Figure S29. Absorption and Emission spectra of BODIPY dye **6** in methanol (excitation wavelength = 490 nm).

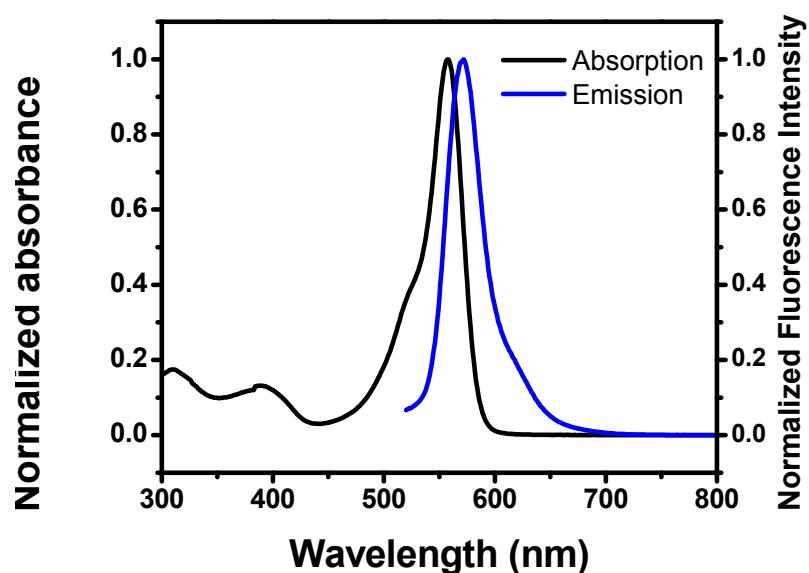


Figure S30. Absorption and Emission spectra of BODIPY dye **7a** in dichloromethane (excitation wavelength = 510 nm).

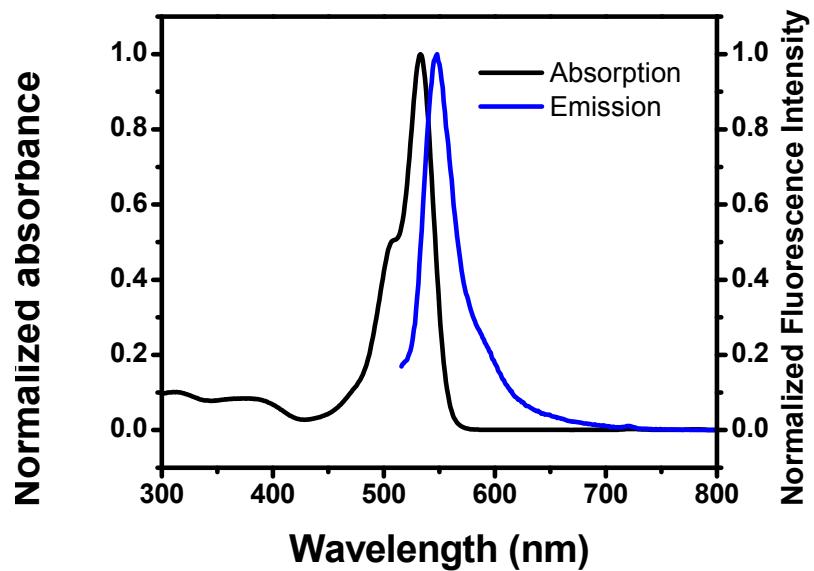


Figure S31. Absorption and Emission spectra of BODIPY dye **7b** in dichloromethane (excitation wavelength = 480 nm).

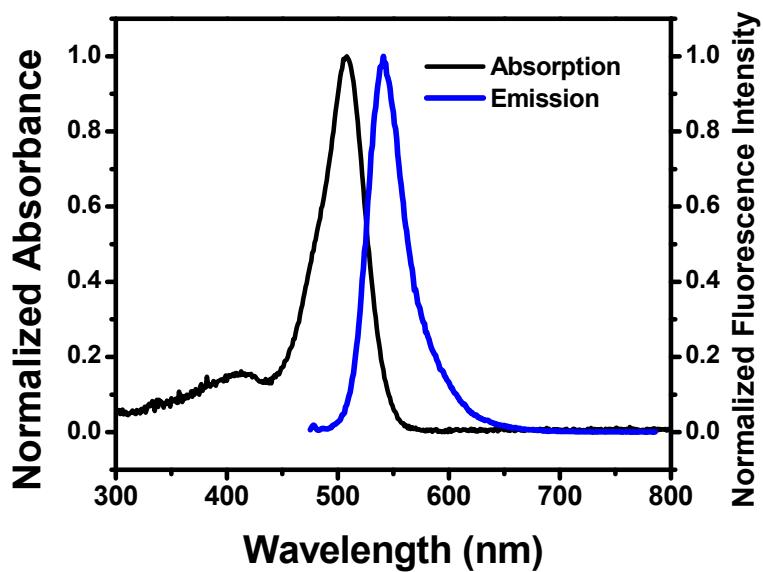


Figure S32. Absorption and Emission spectra of BODIPY dye **8** in dimethyl sulfoxide solution (excitation wavelength = 465 nm).

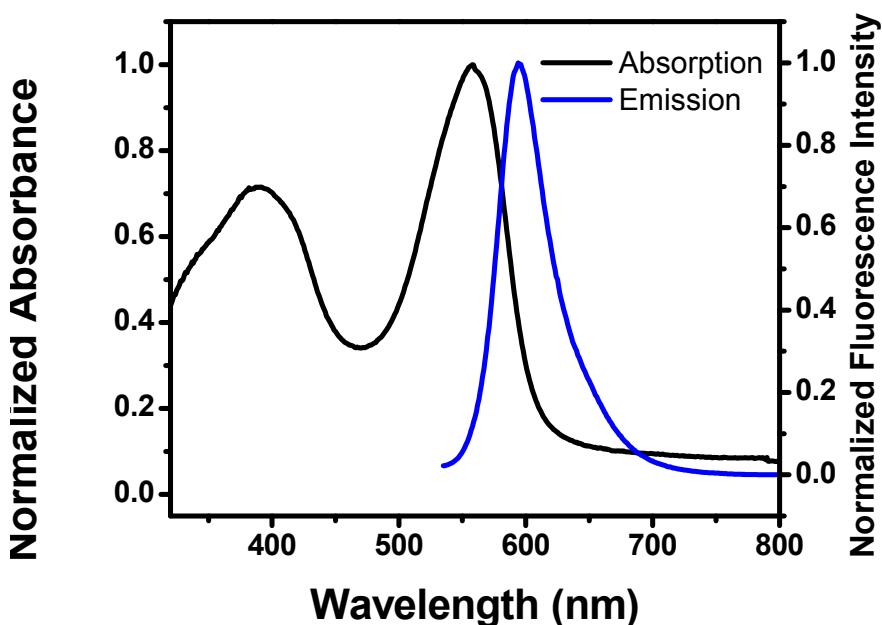


Figure S33. Absorption and Emission spectra of BODIPY dye **10** in dichloromethane solution.
(excitation wavelength = 500 nm)

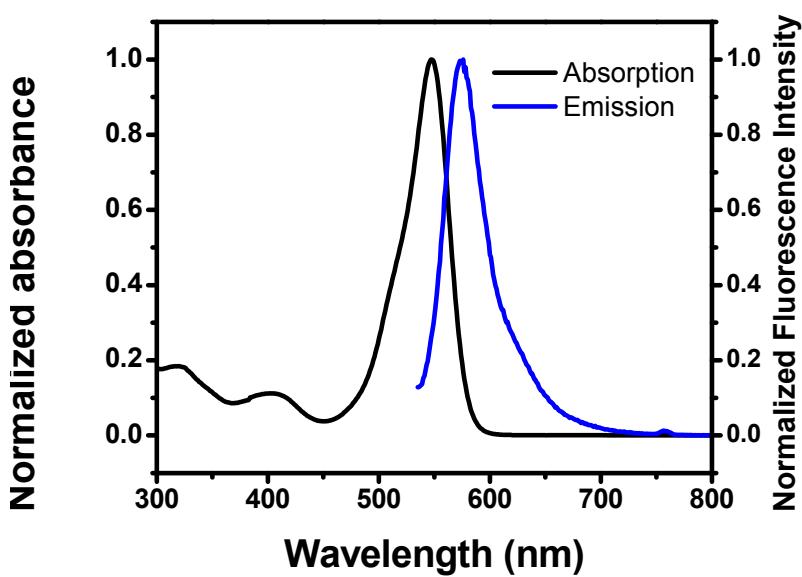


Figure S34. Absorption and Emission spectra of BODIPY dye **11** in dichloromethane (excitation wavelength = 505 nm).

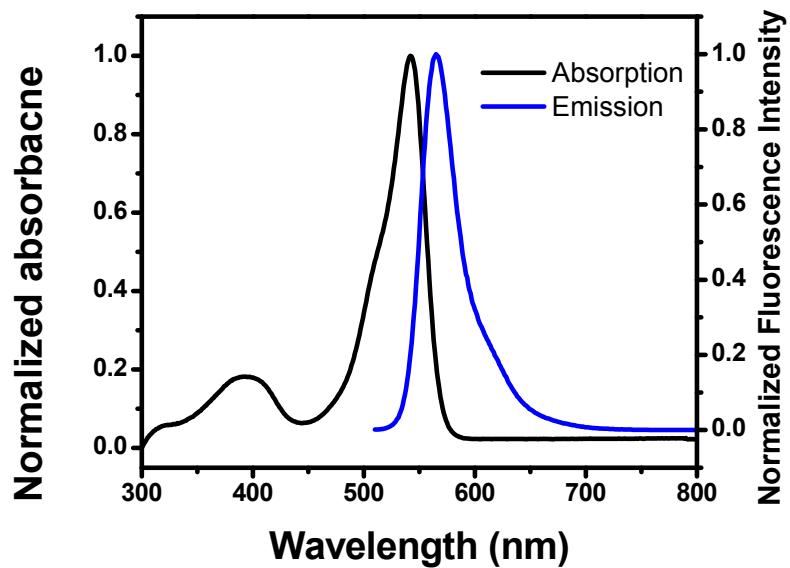


Figure S35. Absorption and Emission spectra of BODIPY dye **12** in dichloromethane (excitation wavelength = 500 nm).

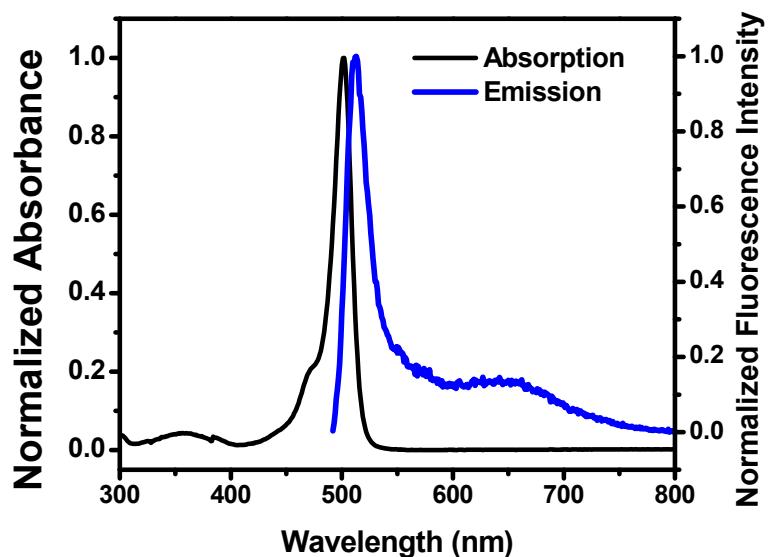


Figure S36. Absorption and Emission spectra of BODIPY dye **13** in dichloromethane solution (excitation wavelength = 470 nm).

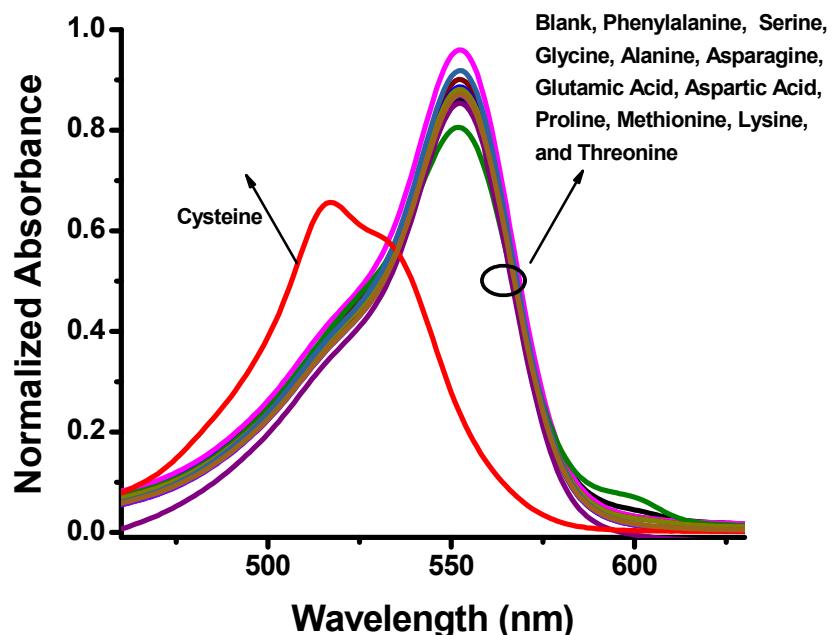


Figure S37. Absorption spectra of BODIPY dye **7a** in the absence and presence of different amounts of cysteine in a mixed solution of acetonitrile and HEPES buffer (pH=7.4) (v/v: 1:1).

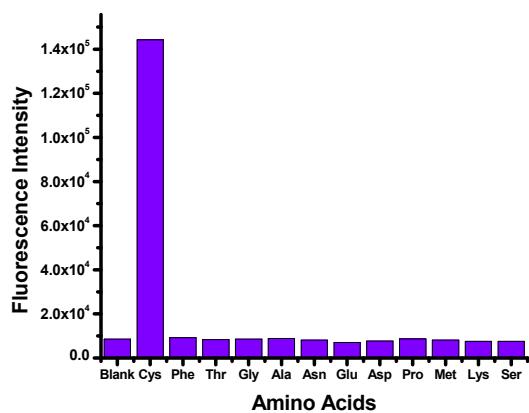


Figure S38. Fluorescence intensity at 527nm of 10 μ M BODPY dye **7a** in the absence and presence of different amino acids (200 equivalents) in a mixed solution of acetonitrile and HEPES buffer (pH 7.4) (v/v: 1:1)

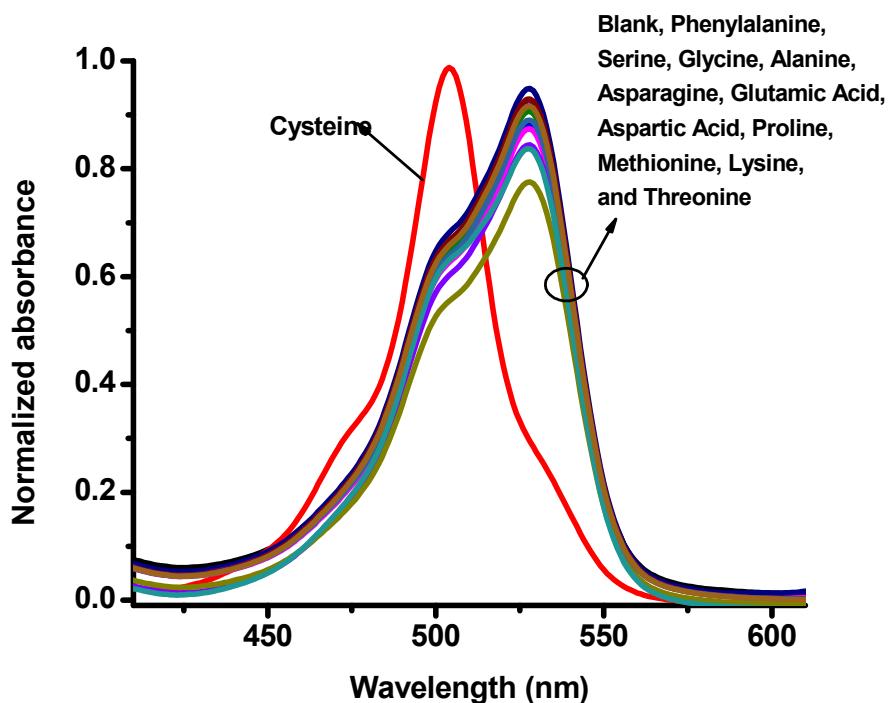


Figure S39. Absorption spectra of BODIPY dye **7b** in the absence and presence of different amino acids in a mixed solution of acetonitrile and HEPES buffer (pH=7.4) (v/v: 1:1).

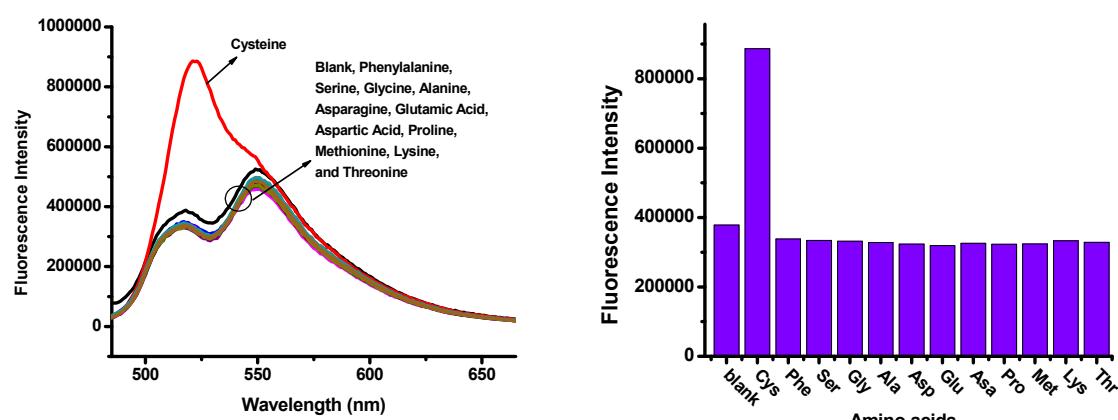


Figure S40. Fluorescence spectra (left) and fluorescence intensity at 521nm (right) of 10 μ M BODPY dye **7b** in the absence and presence of different amino acids (200 equivalents) in a mixed of acetonitrile and HEPES buffer (pH 7.4) (1:1) .

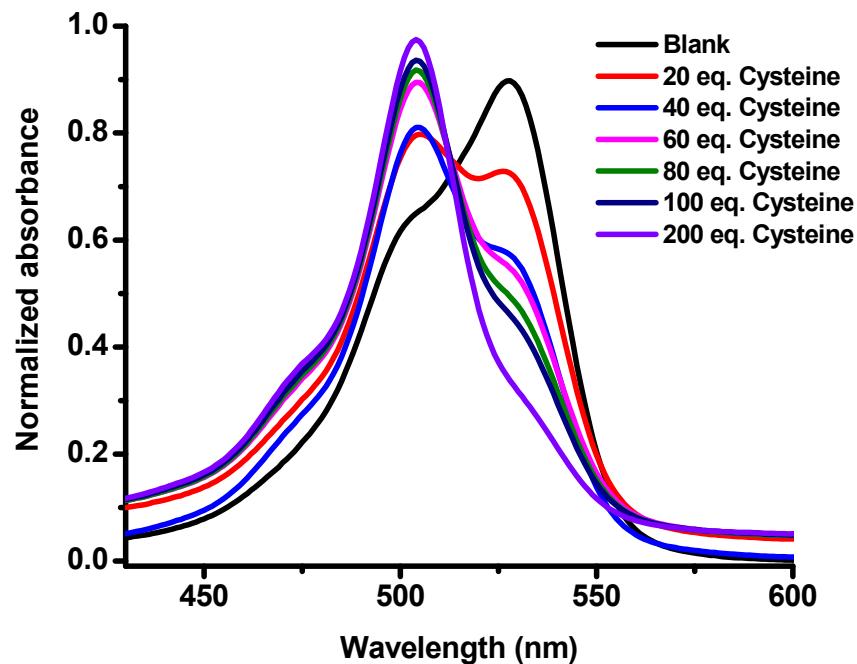


Figure S41. Absorption spectra of BODIPY dye **7b** in the absence and presence of different amounts of cysteine in a mixed solution of acetonitrile and HEPES buffer (pH=7.4) (v/v: 1:1).

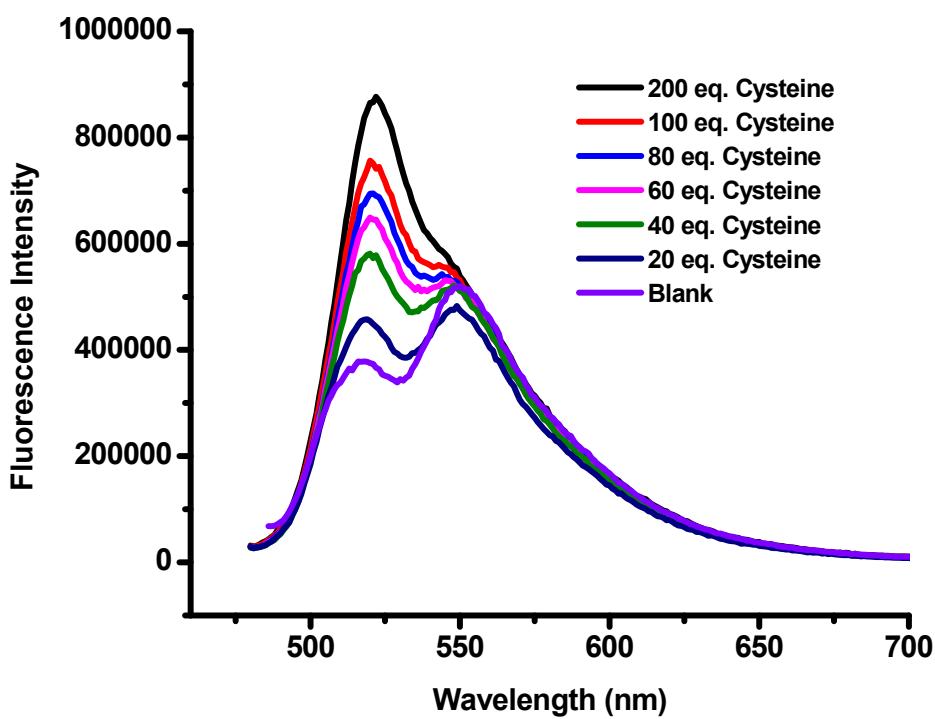
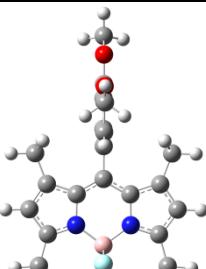
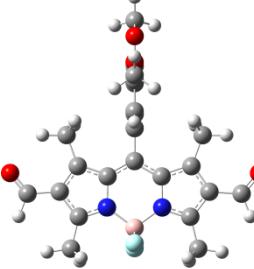
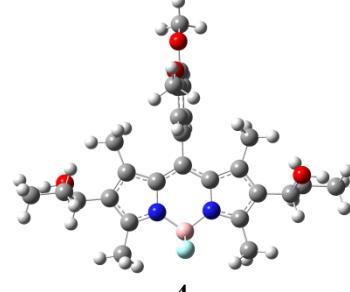
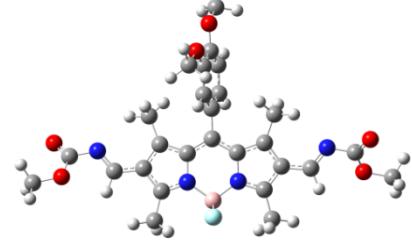
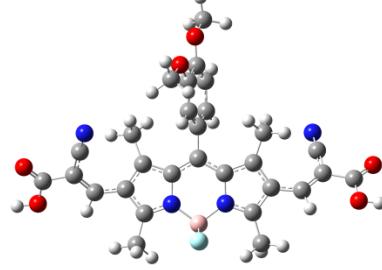
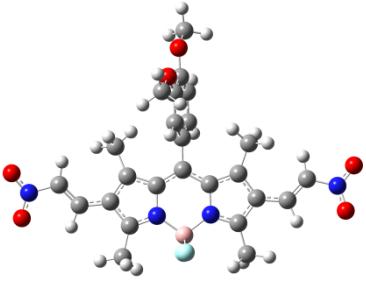
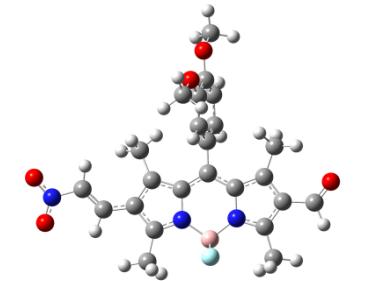
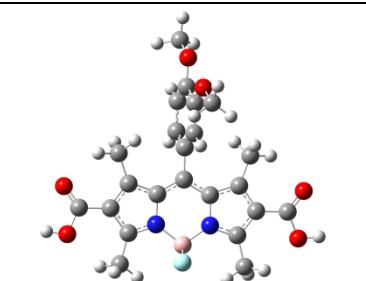
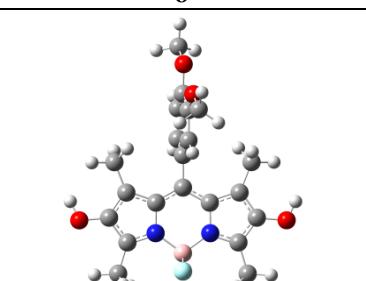
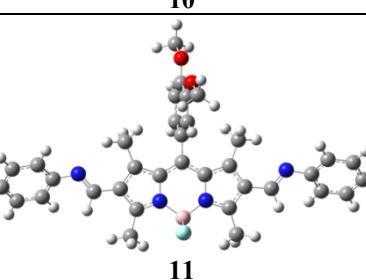
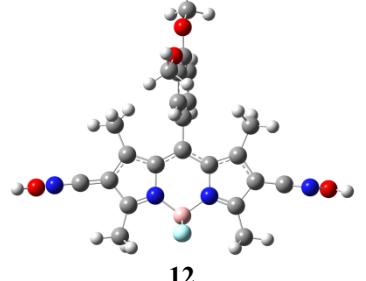


Figure S42. Fluorescence spectra of BODIPY dye **7b** in the absence and presence of different amounts of cysteine in a mixed solution of acetonitrile and HEPES buffer (pH=7.4) (v/v: 1:1).

Table S1. Energies (in Hartree) for the HOMO/LUMO levels as obtained at B3LYP/6-311G(d,p) level of theory for the coupled and uncoupled Aryl/BODIPY structures. The latter should be compared with the HOMO and LUMO level of the standalone benzene moiety (as reported graphically in Figure 4 of the main text) which lie at -0.22615 au and -0.01123 au, respectively. Also reported are the quantum yields obtained experimentally.

BODIPY dye	Computed Energies --Coupled Structures		Computed Energies --Uncoupled Structures		Quantum Yield (%)
	HOMO	LUMO	HOMO	LUMO	
 1	-0.21081	-0.09974	-0.21129	-0.10199	68
 3	-0.22293	-0.12050	-0.23336	-0.12175	0.60
 4	-0.20914	-0.09962	-0.21005	-0.10114	87
 5	-0.22293	-0.12089	-0.23104	-0.12219	8.7%
 6	-0.22357	0.12442	-0.22992	-0.12625	1.9

 7a	-0.22567	-0.12754	-0.23075	-0.12936	12
 7b	-0.22453	-0.12410	-0.23197	-0.12590	1.3
 8	-0.22232	-0.11440	-0.22947	-0.11554	1.0
 10	-0.19851	-0.09959	-0.19778	-0.09946	7.6
 11	-0.21552	-0.11345	-0.21675	-0.11486	0.23
 12	-0.15641	-0.10938	-0.15785	-0.10980	47

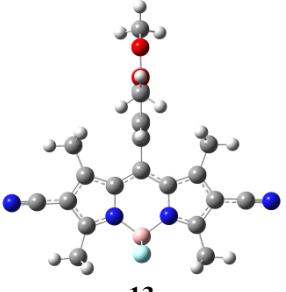
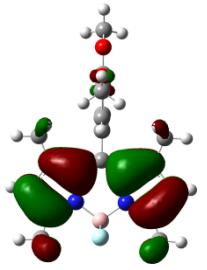
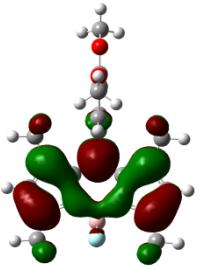
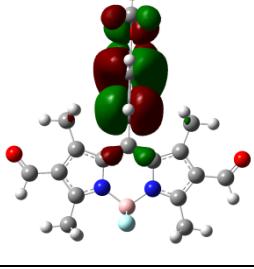
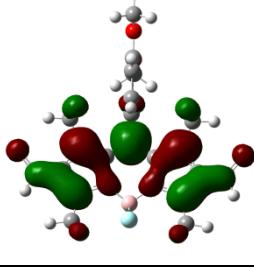
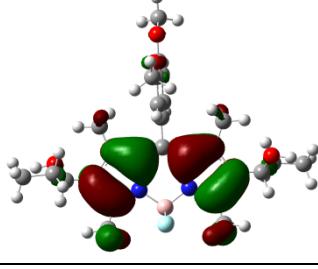
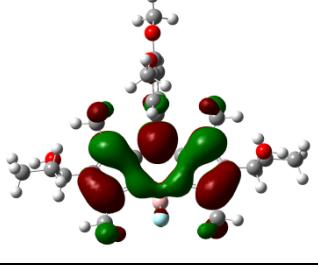
 13	-0.22523	-0.12315	-0.23769	-0.12565	0.08
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Table S2. HOMO/LUMO level charge distributions as obtained at B3LYP/6-311G(d,p) level of theory for the coupled Aryl/BODIPY structures.

BODIPY Dye	HOMO	LUMO
1		
3		
4		
5	