

Carbazole Substituted Boron Dipyrromethenes

Praseetha E. Kesavan^a, Iti Gupta^{*a}

^aIndian Institute of Technology Gandhinagar, VGEC Campus, Chandkheda, Ahmedabad-382424, India

List of Contents

Figure 1: HRMS Spectrum of <i>meso</i> -N-butylcarbazoledipyrromethane.	S3
Figure 2: ¹ H NMR spectrum of <i>meso</i> -N-butylcarbazoledipyrromethane in CDCl ₃ .	S3
Figure 3: ¹³ C NMR of carbazole DPM in CDCl ₃ .	S4
Figure 4: HRMS Spectrum of BODIPY 1.	S4
Figure 5: ¹ H NMR spectrum of BODIPY 1 recorded in CDCl ₃ .	S5
Figure 6: ¹³ C NMR spectrum of BODIPY 1 recorded in CDCl ₃ .	S5
Figure 7: COSY of BODIPY 1 recorded in CDCl ₃ .	S6
Figure 8: ¹⁹ F NMR of BODIPY 1 recorded in CDCl ₃ .	S6
Figure 9: HRMS Spectrum of BODIPY 2.	S7
Figure 10: ¹ H NMR spectrum of BODIPY 2 recorded in CDCl ₃ .	S7
Figure 11: ¹³ C NMR spectrum of BODIPY 2 recorded in CDCl ₃ .	S8
Figure 12: COSY of BODIPY 2 recorded in CDCl ₃ .	S8
Figure 13: ¹⁹ F NMR of BODIPY 2 recorded in CDCl ₃ .	S9
Figure 14: HRMS Spectrum of BODIPY 3.	S9
Figure 15: ¹ H NMR spectrum of BODIPY 3 recorded in CDCl ₃ .	S10
Figure 16: ¹³ C NMR spectrum of BODIPY 3 recorded in CDCl ₃ .	S10
Figure 17: COSY of BODIPY 3 recorded in CDCl ₃ .	S11
Figure 18: ¹⁹ F NMR of BODIPY 3 recorded in CDCl ₃ .	S11
Figure 19: HRMS Spectrum of BODIPY 4.	S12

Figure 20: ^1H NMR spectrum of BODIPY 4 recorded in CDCl_3 .	S12
Figure 21: ^{13}C NMR spectrum of BODIPY 4 recorded in CDCl_3 .	S13
Figure 22: COSY of BODIPY 4 recorded in CDCl_3 .	S13
Figure 23: ^{19}F NMR of BODIPY 4 recorded in CDCl_3 .	S14
Figure 24: Comparison of emission spectra of BODIPY 1-4 and N-butylcarbazole excited at 347nm in CHCl_3 .	S14
Figure 25: Decay profile and weighted, residual, distribution fit of BODIPY 1-4	S15
Table 1: Selected bond distances (\AA) and bond angles ($^\circ$) for BODIPYs 1 and 2 .	S15
Figure 26: Absorption spectra of BODIPY 1-4 in different solvents.	S16
Figure 27: Emission spectra of BODIPY 1-4 in different solvents	S17

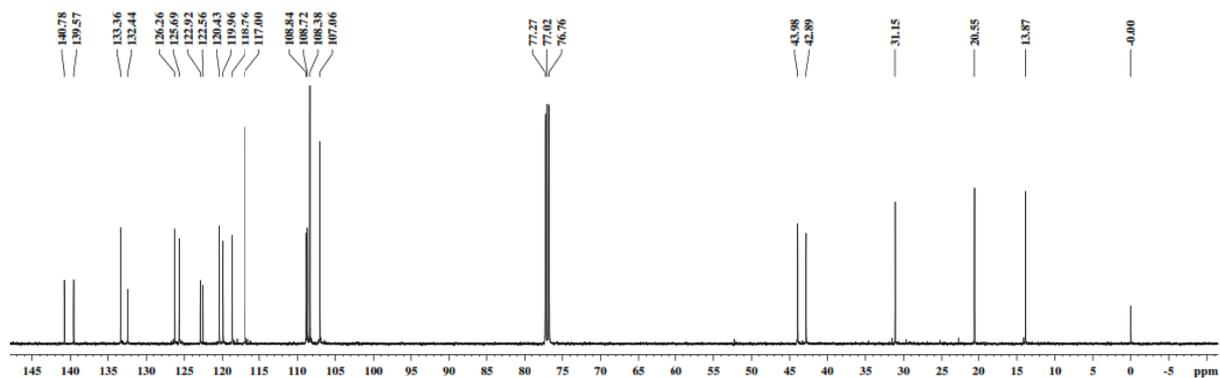


Figure 3: ^{13}C NMR of carbazole DPM recorded in CDCl_3 .

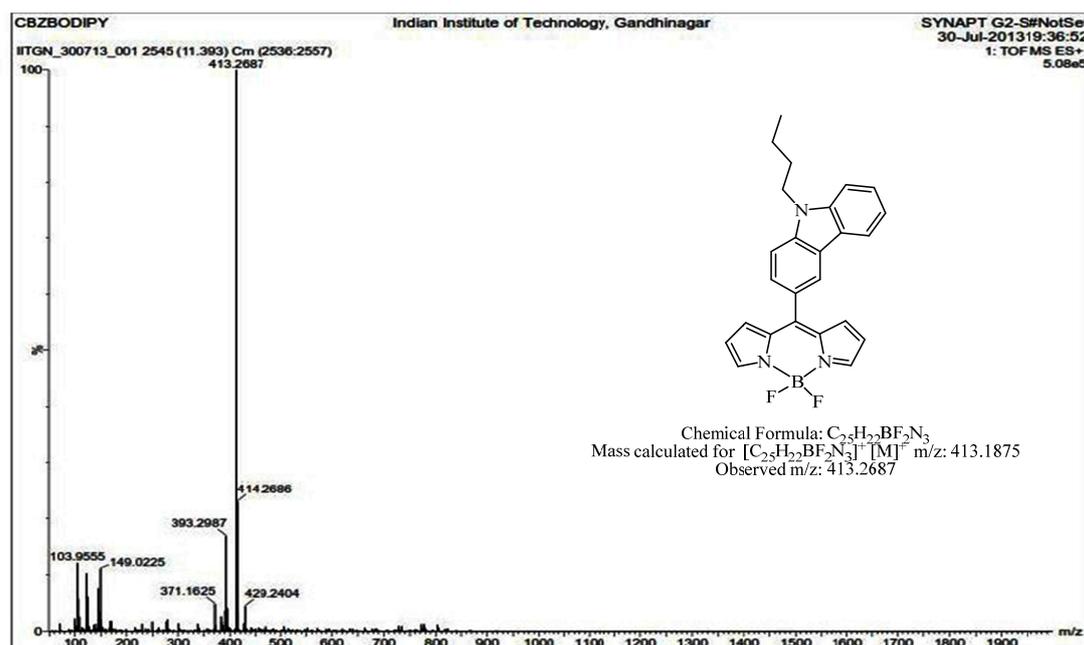


Figure 4: HRMS Spectrum of BODIPY 1.

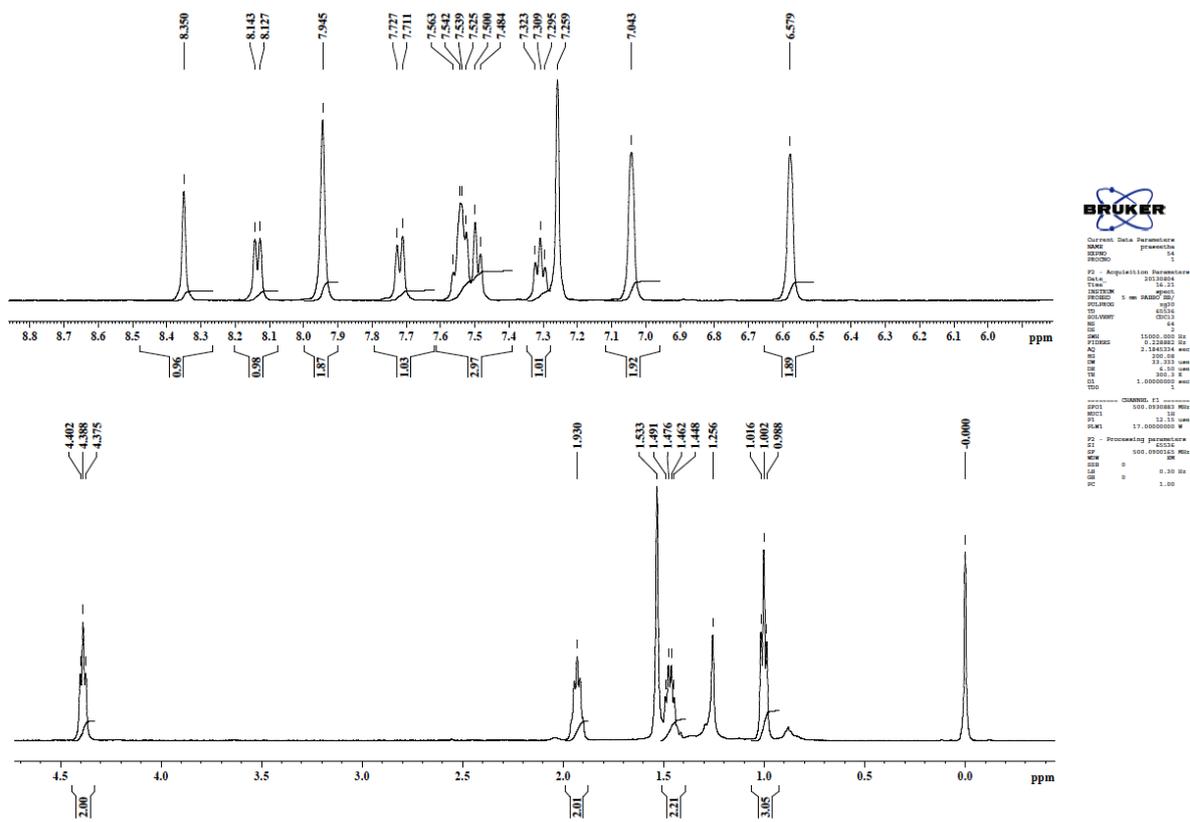


Figure 5: ^1H NMR spectrum of BODIPY 1 recorded in CDCl_3 .

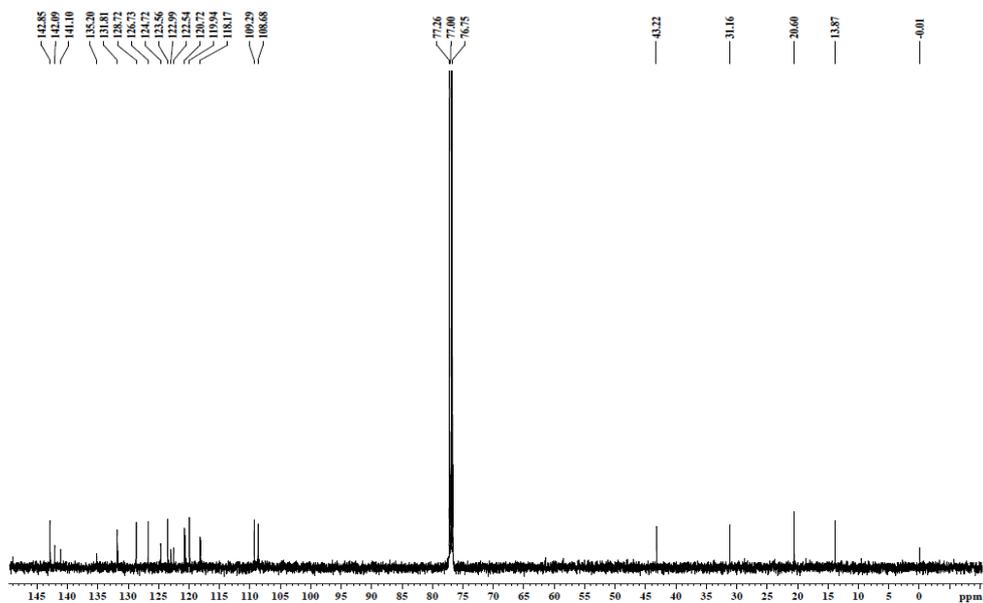


Figure 6: ^{13}C NMR spectrum of BODIPY 1 recorded in CDCl_3 .

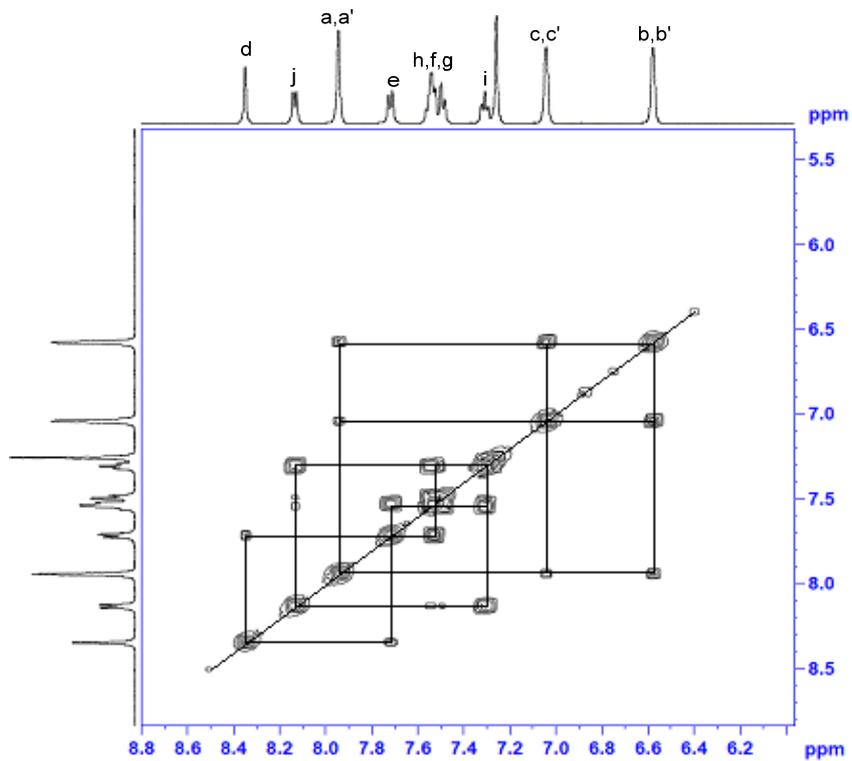


Figure 7: COSY of BODIPY **1** recorded in CDCl₃.

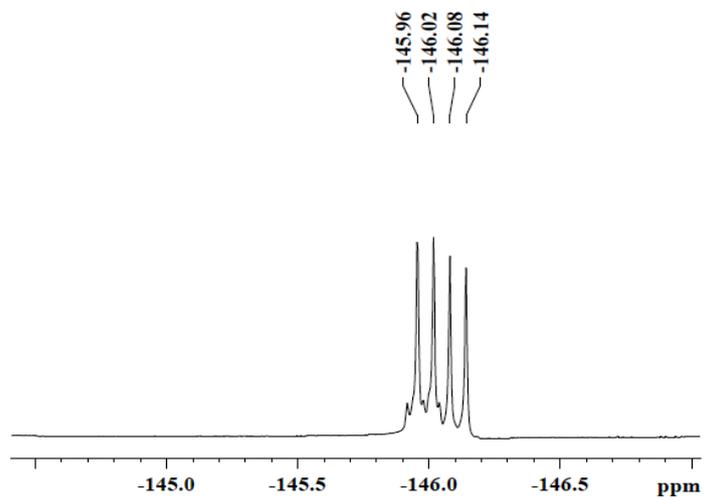


Figure 8: ¹⁹F NMR of BODIPY **1** recorded in CDCl₃.

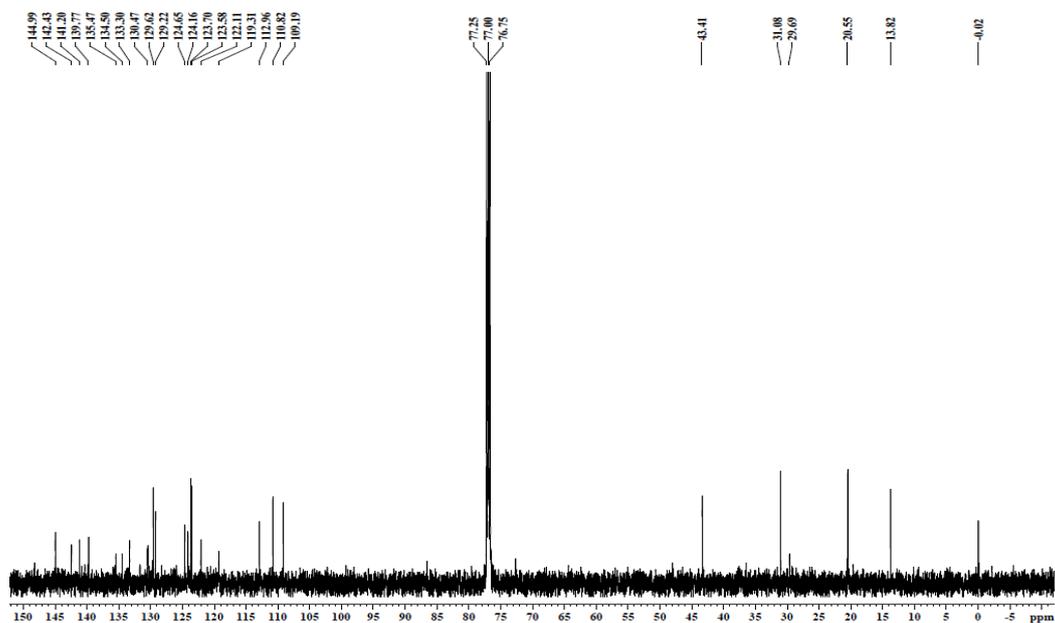


Figure 11: ^{13}C NMR spectrum of BODIPY 2 recorded in CDCl_3 .

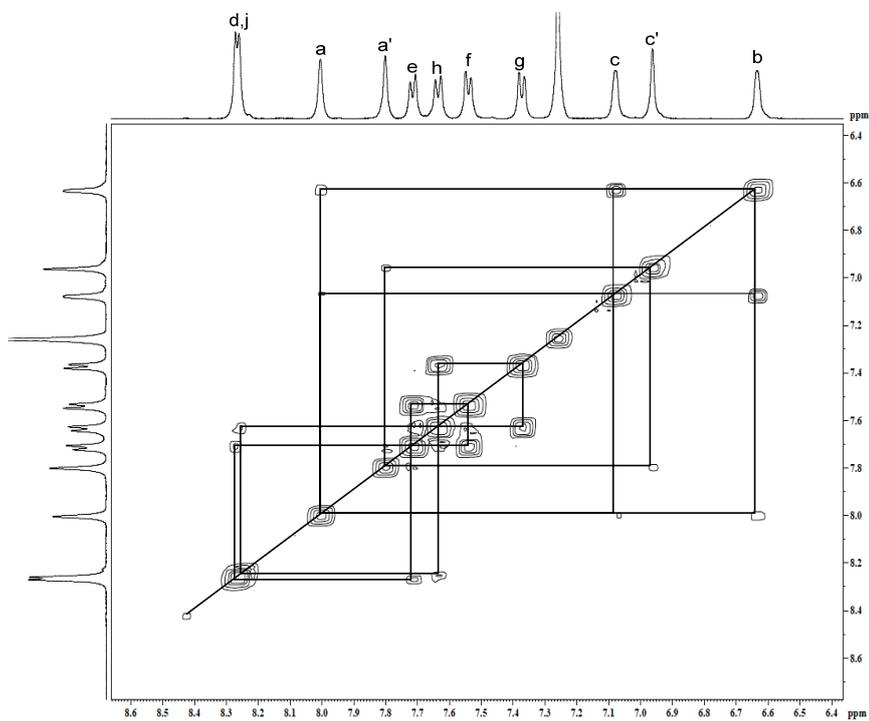


Figure 12: COSY of BODIPY 2 recorded in CDCl_3 .

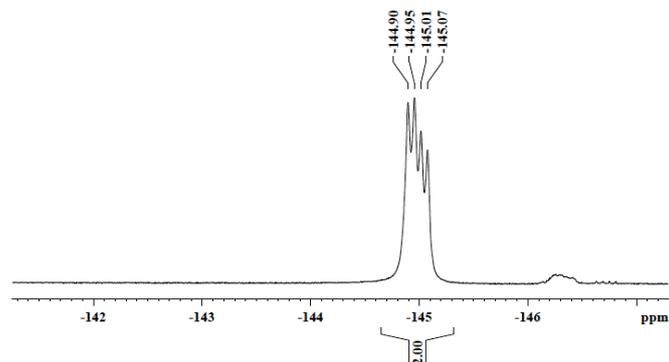


Figure 13: ^{19}F NMR of BODIPY 2 recorded in CDCl_3 .

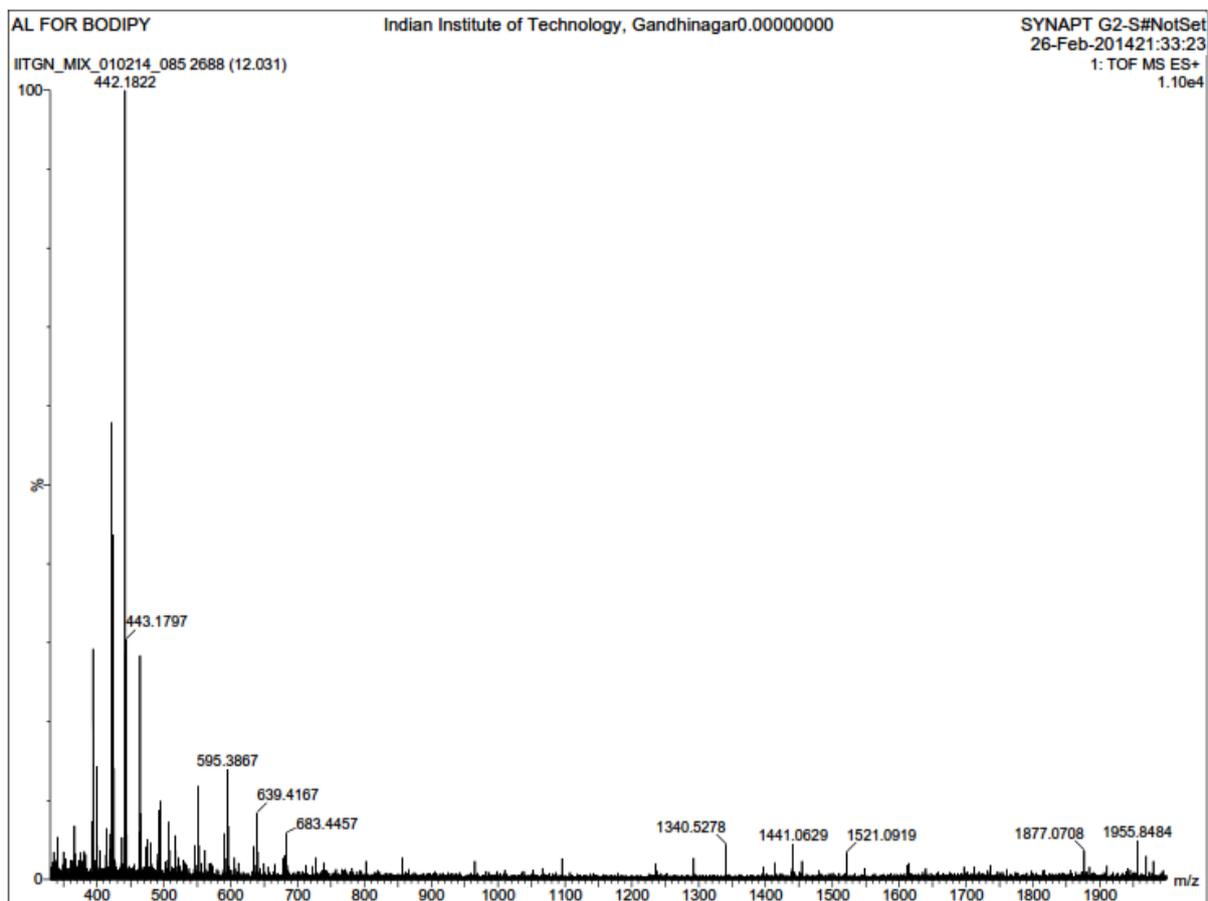


Figure 14: HRMS Spectrum of BODIPY 3.

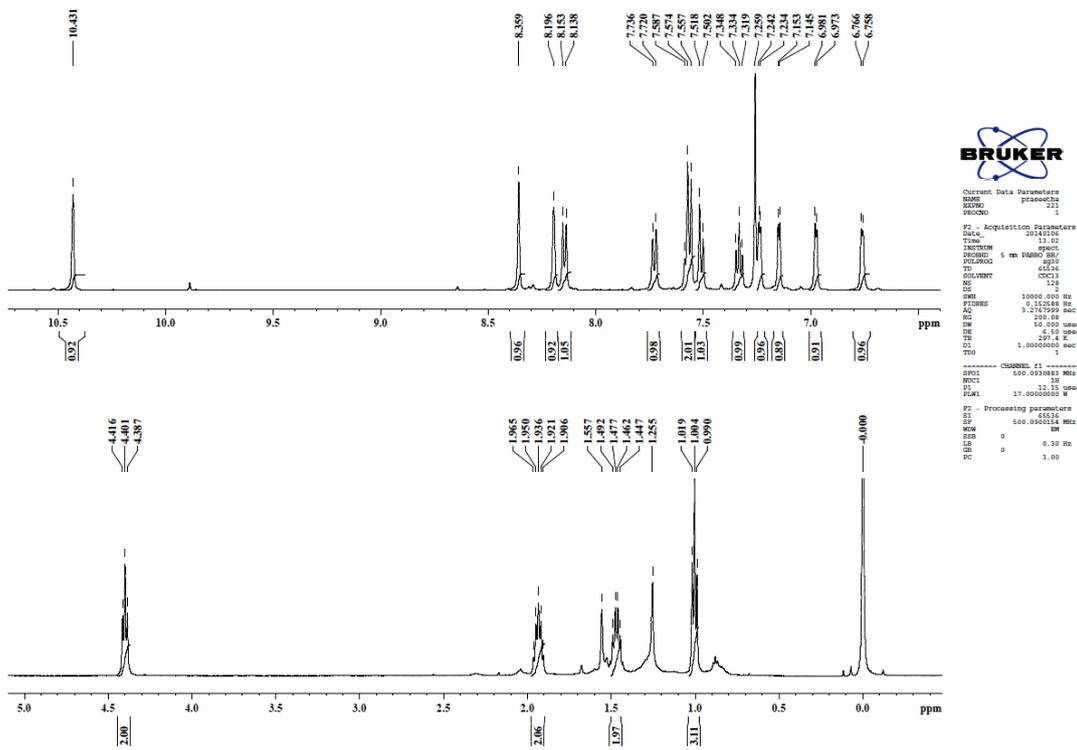


Figure 15: ¹H NMR spectrum of BODIPY 3 recorded in CDCl₃.

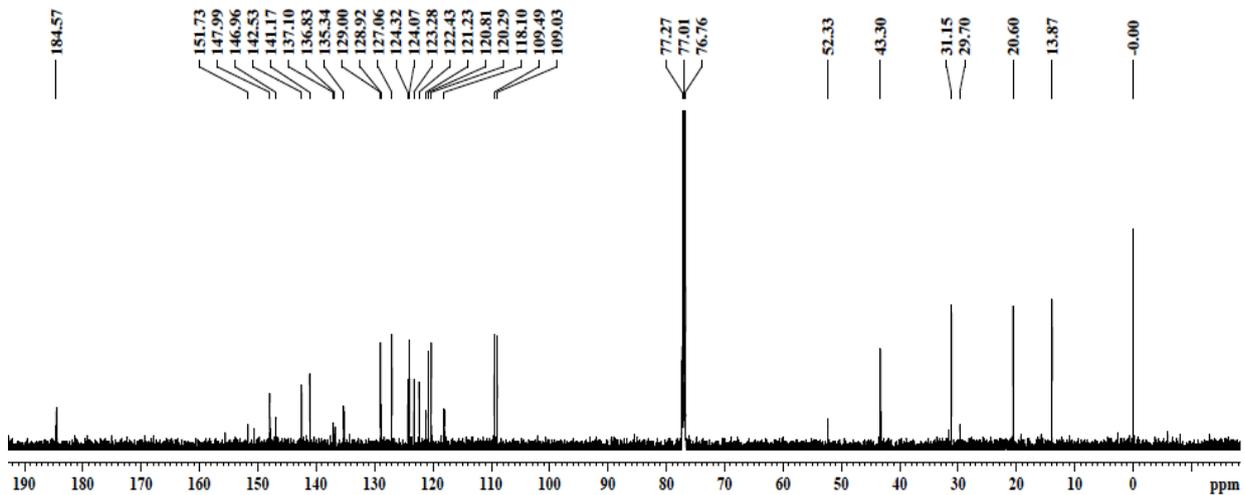


Figure 16: ¹³C NMR spectrum of BODIPY 3 recorded in CDCl₃.

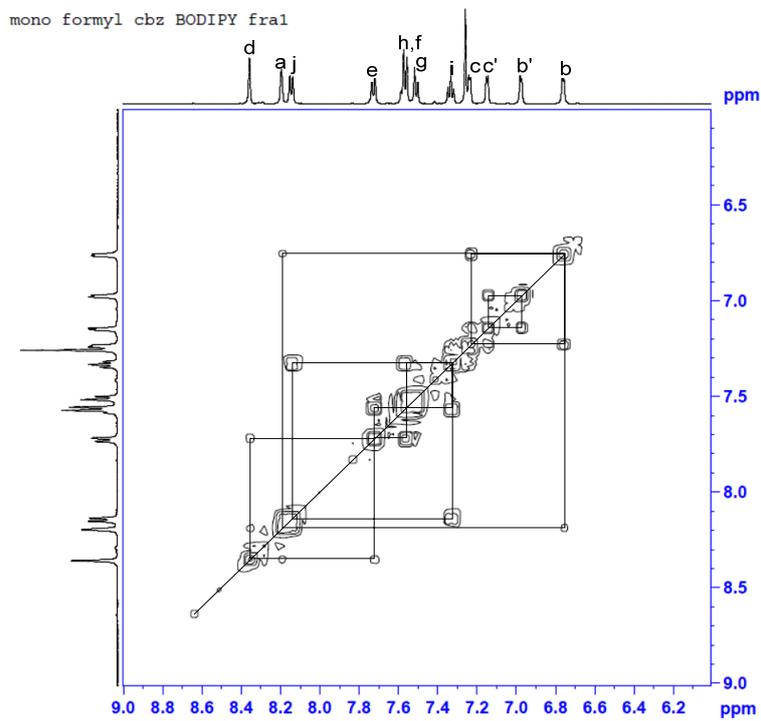


Figure 17: COSY of BODIPY 3 recorded in CDCl_3 .

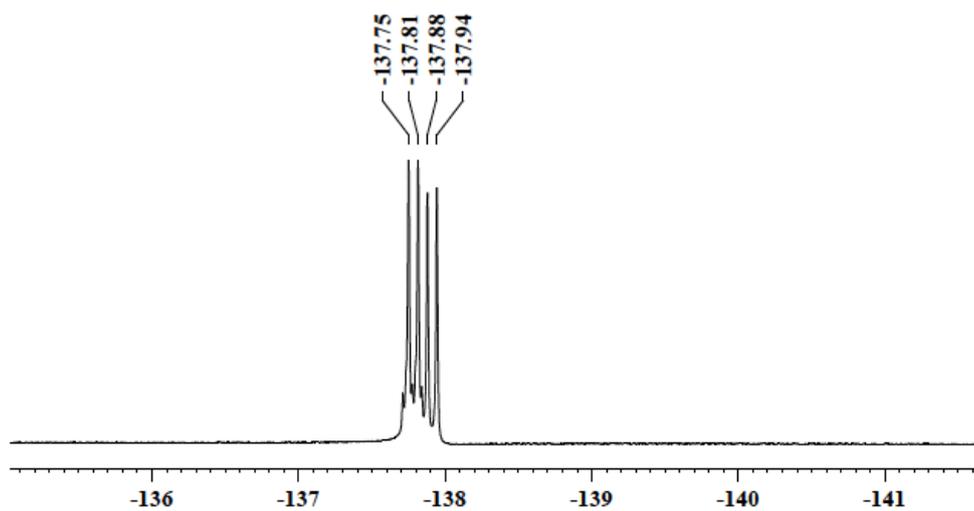


Figure 18: ^{19}F NMR of BODIPY 3 recorded in CDCl_3 .

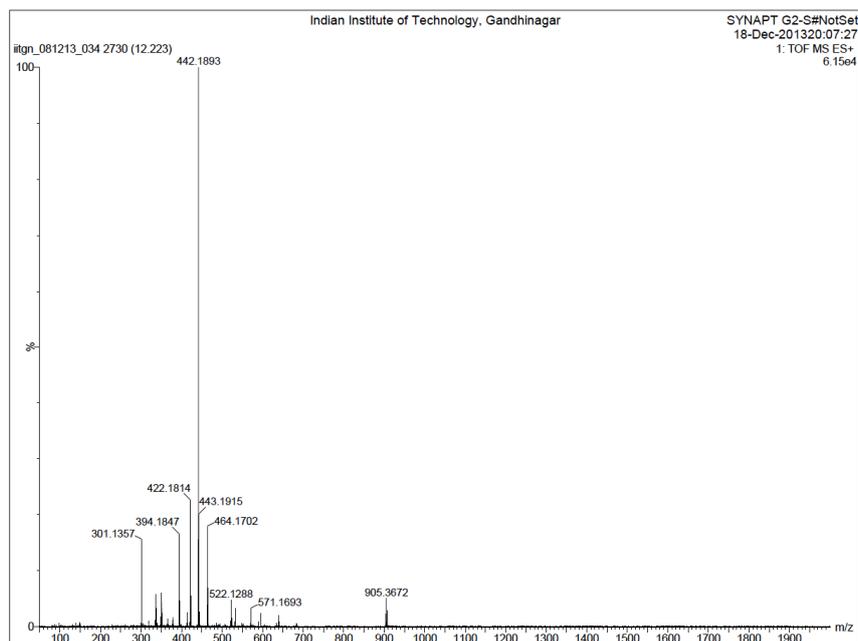


Figure 19: HRMS Spectrum of BODIPY 4.

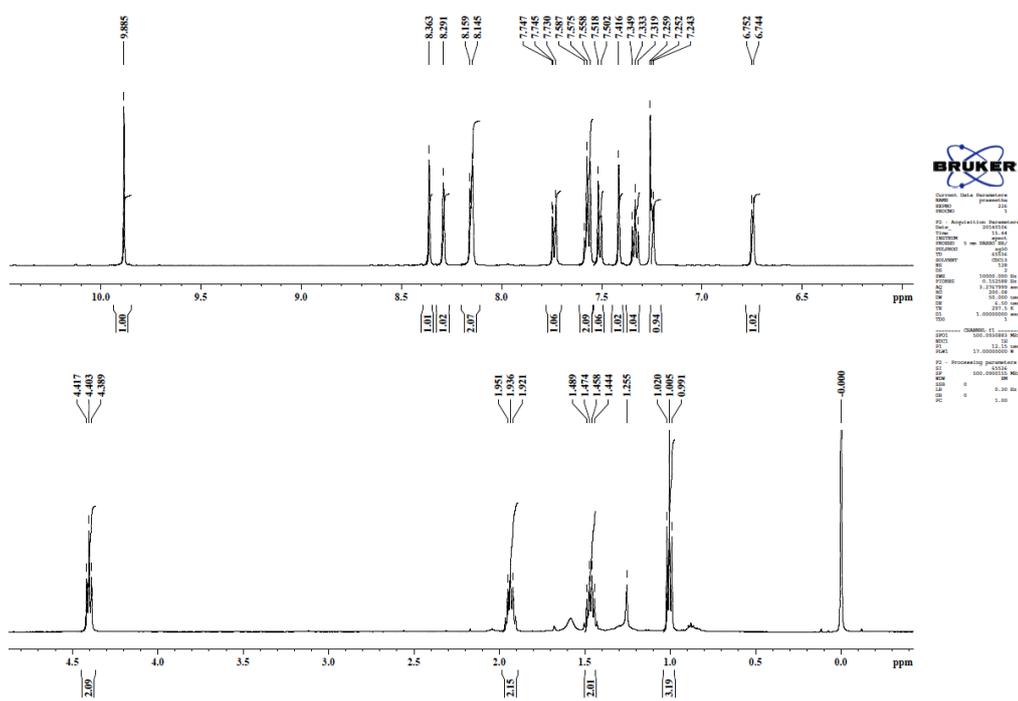


Figure 20: ¹H NMR spectrum of BODIPY 4 recorded in CDCl₃.

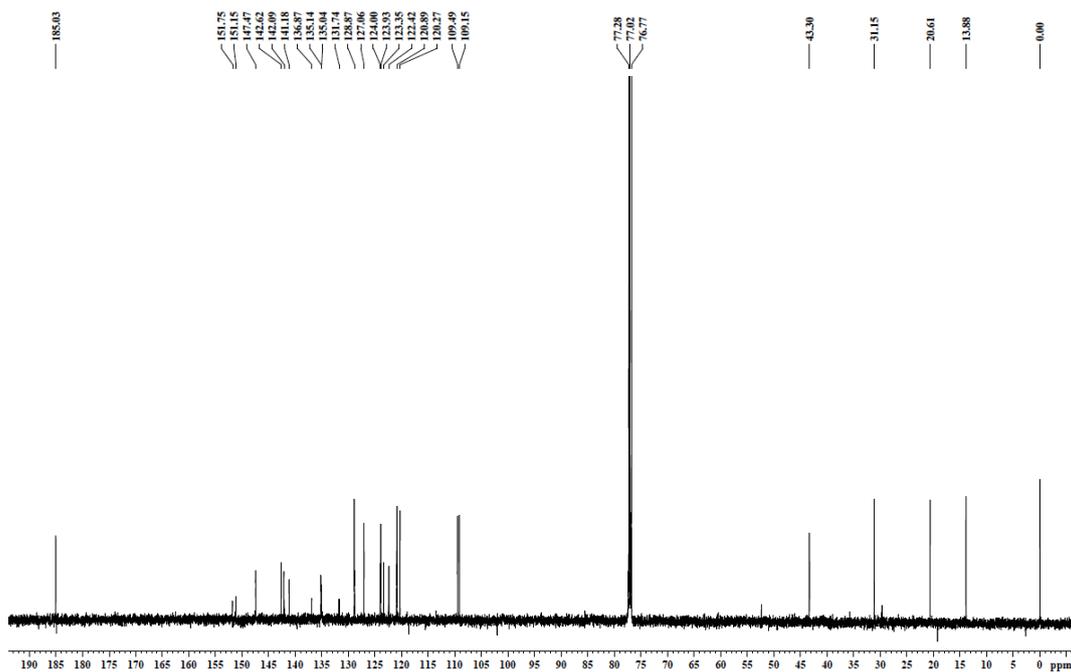


Figure 21: ^{13}C NMR spectrum of BODIPY **4** recorded in CDCl_3 .

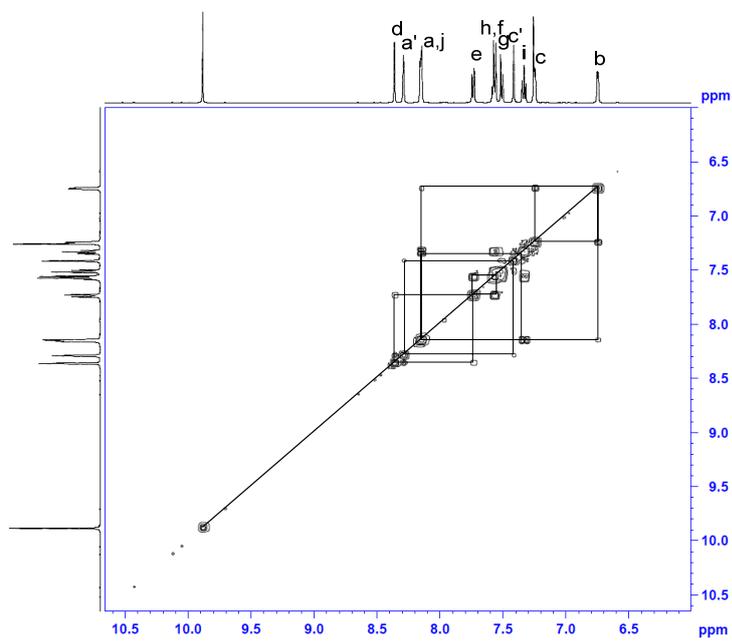


Figure 22: COSY of BODIPY **4** recorded in CDCl_3 .

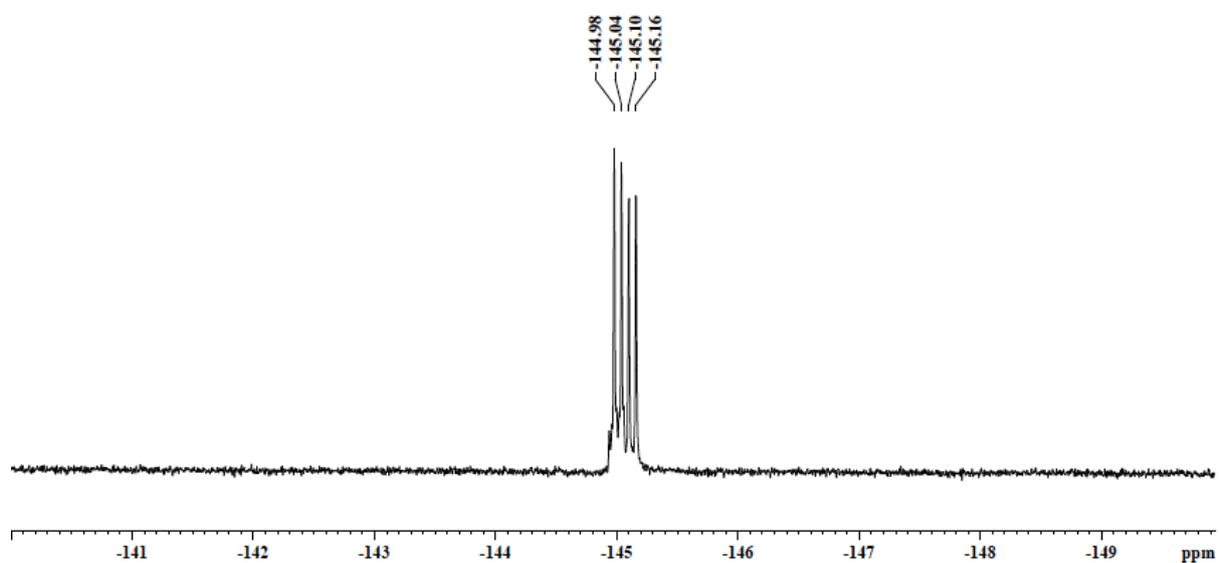


Figure 23: ^{19}F NMR of BODIPY 4 recorded in CDCl_3 .

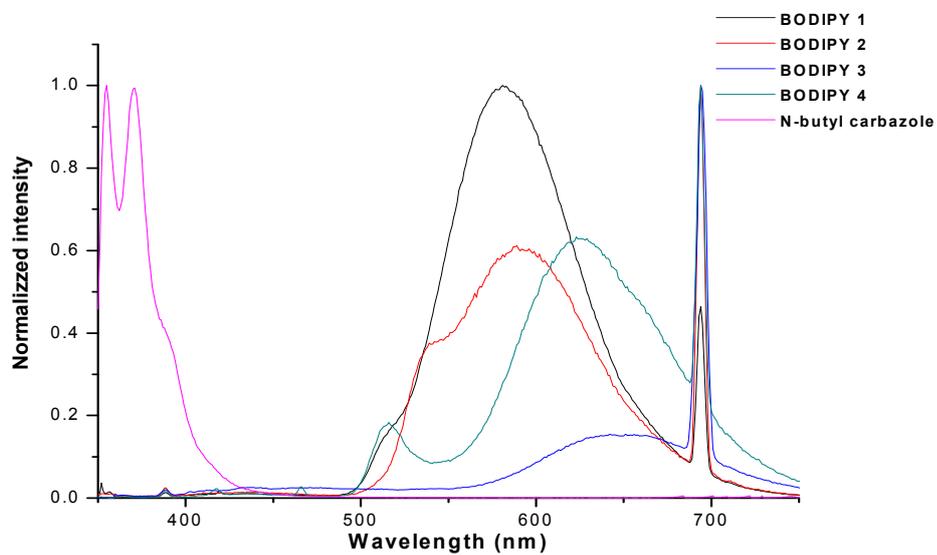


Figure 24: Comparison of emission spectra of BODIPY 1-4 and N-butylcarbazole excited at 347nm, recorded in CHCl_3 .

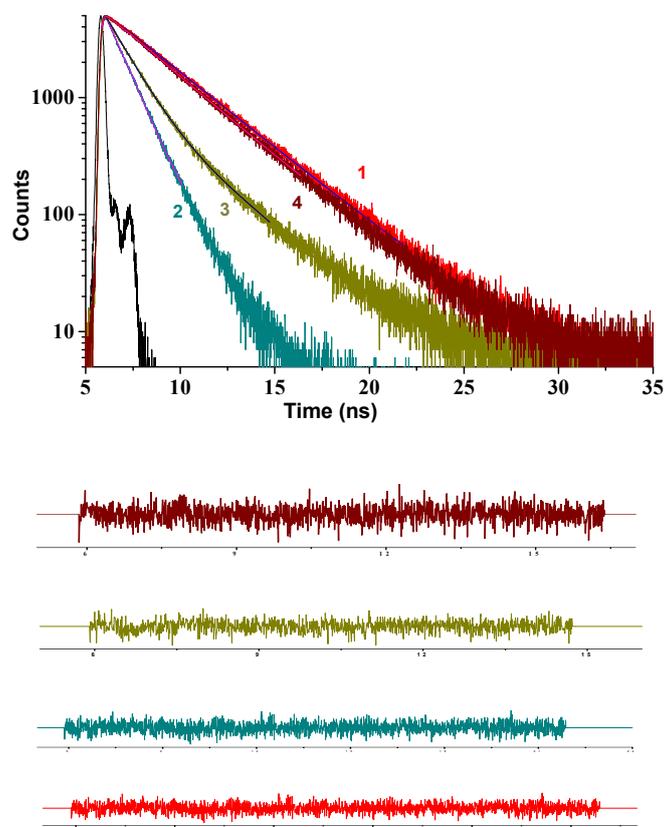


Figure 25: Fluorescence decay profile and weighted, residual, distribution fit of BODIPY1-4 in chloroform. The excitation wavelength used was 440 nm and emission detected at corresponding wavelengths.

Table 1: Selected bond distances (Å) and bond angles ($^{\circ}$) for **BODIPYs 1 and 2**.

Bond length/torsion angles	BODIPY 1	BODIPY 2
B1-F1	1.392(19)	1.39(2)
B2-F2	1.393(18)	1.372(18)
B1-N1	1.5464(19)	1.58(2)
N1-C1	1.3444(16)	1.341(19)
N1-C4	1.3956(16)	1.393(18)
F1-B1-F2	108.69(11)	107.6(12)
N1-B1-N2	106.03(10)	106.4(12)
C6-C5-C13-C14	46.10(17)	46.7(16)
C4-C5-C13-C12	48.96(18)	46.5(15)
C5-C13	1.474(16)	1.442(17)
C1(α)-C2(β)	1.394(19)	1.30(3)
C2 (β)-C3(β)	1.384(17)	1.39(2)

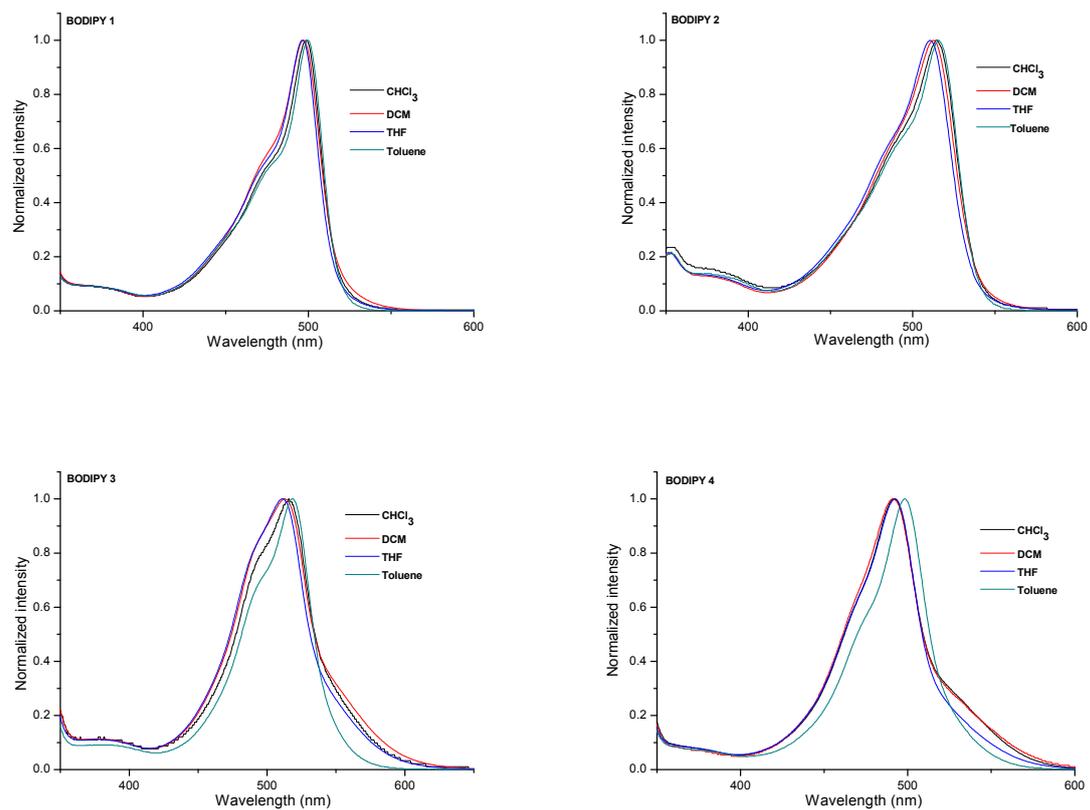


Figure 26: Absorption spectra of BODIPY 1-4 in different solvents.

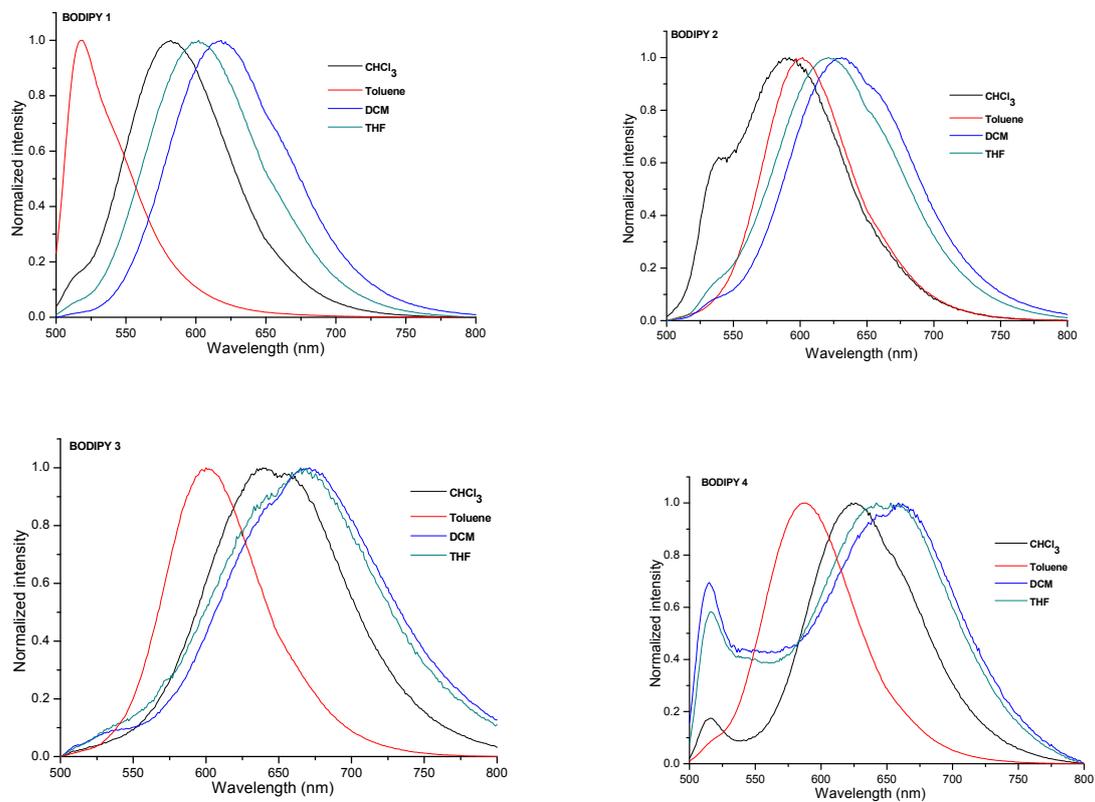


Figure 27: Emission spectra of BODIPY 1-4 in different solvents.
