

## Supplementary information for

### BODIPY Derivatives Modified with Carborane Clusters: Synthesis, Characterization and DFT

#### Studies

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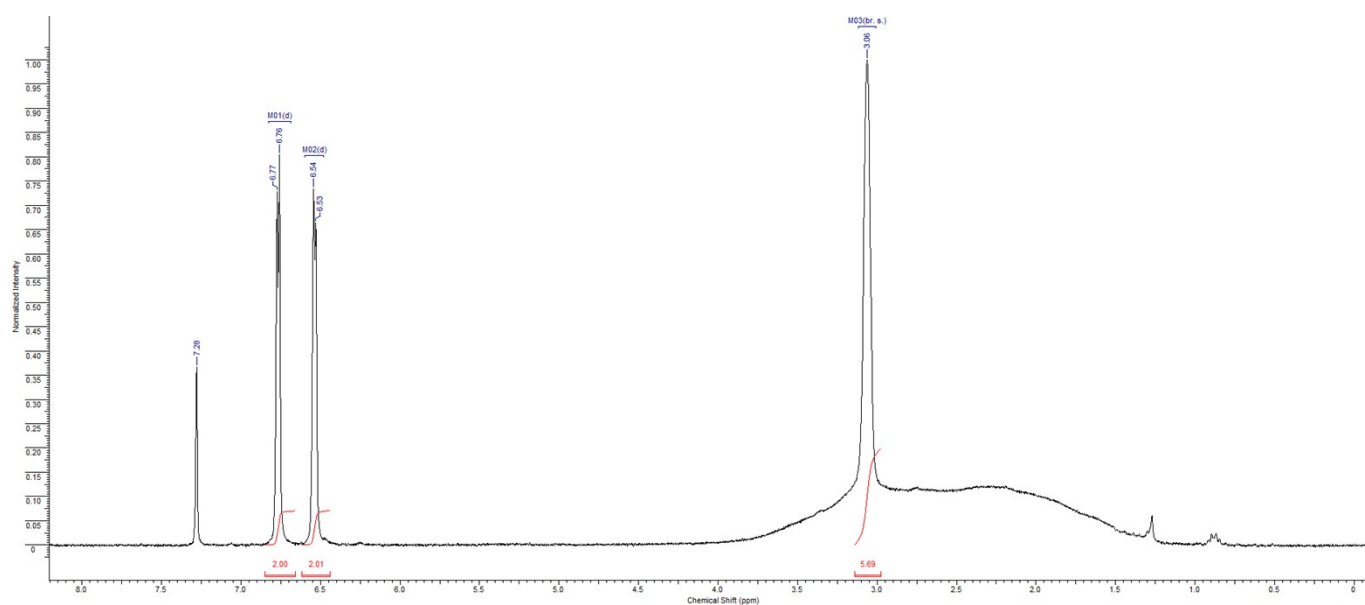


Figure S1.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectrum of compound **4**.

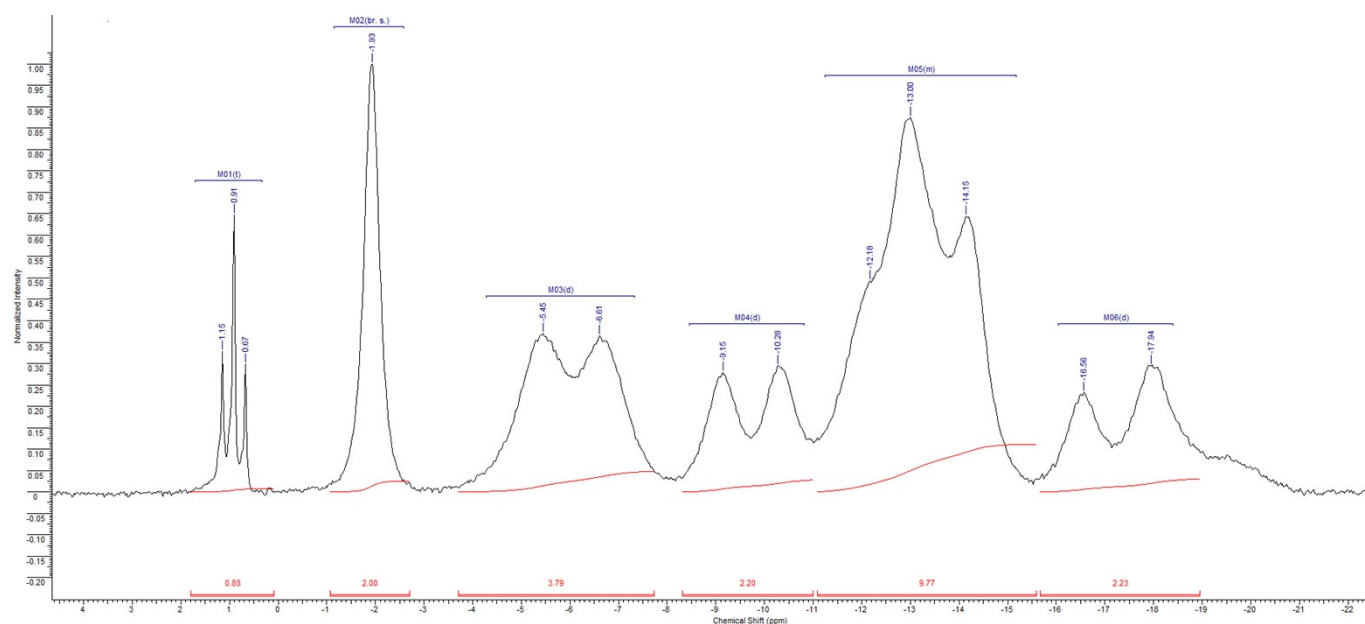


Figure S2.  $^{11}\text{B}$  NMR (128 MHz,  $\text{CDCl}_3$ ) spectrum of compound **4**

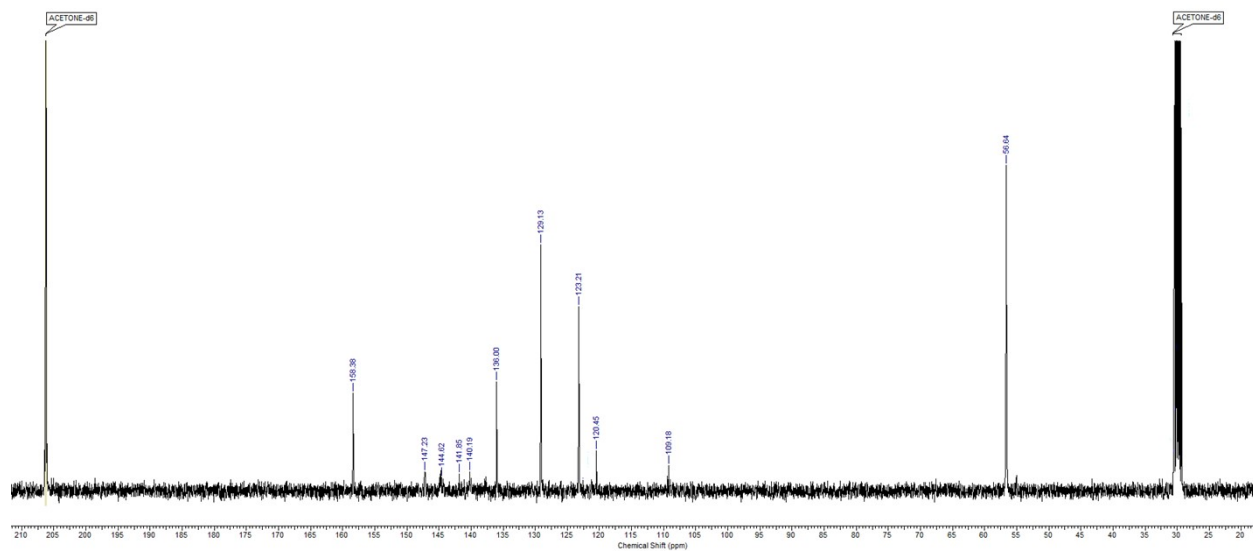


Figure S3.  $^{13}\text{C}$  NMR (100.6 MHz,  $(\text{CD}_3)_2\text{CO}$ ) spectrum of compound 4

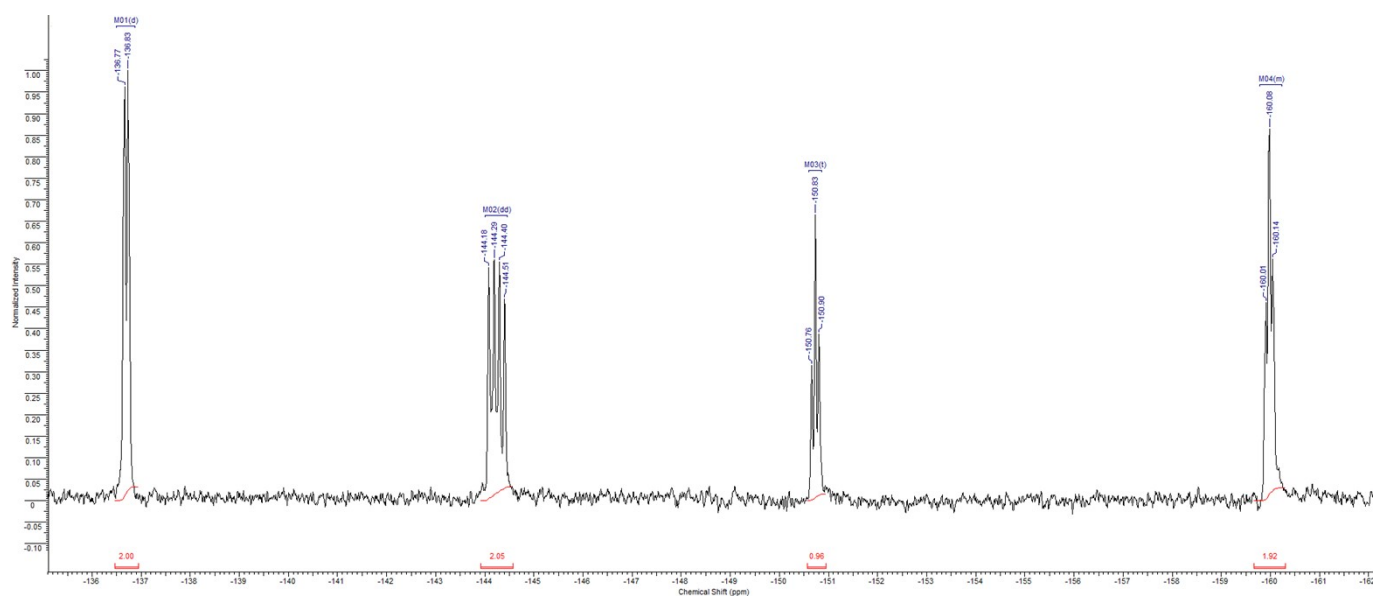


Figure S4.  $^{19}\text{F}$  NMR (282 MHz,  $\text{CDCl}_3$ ) spectrum of compound 4

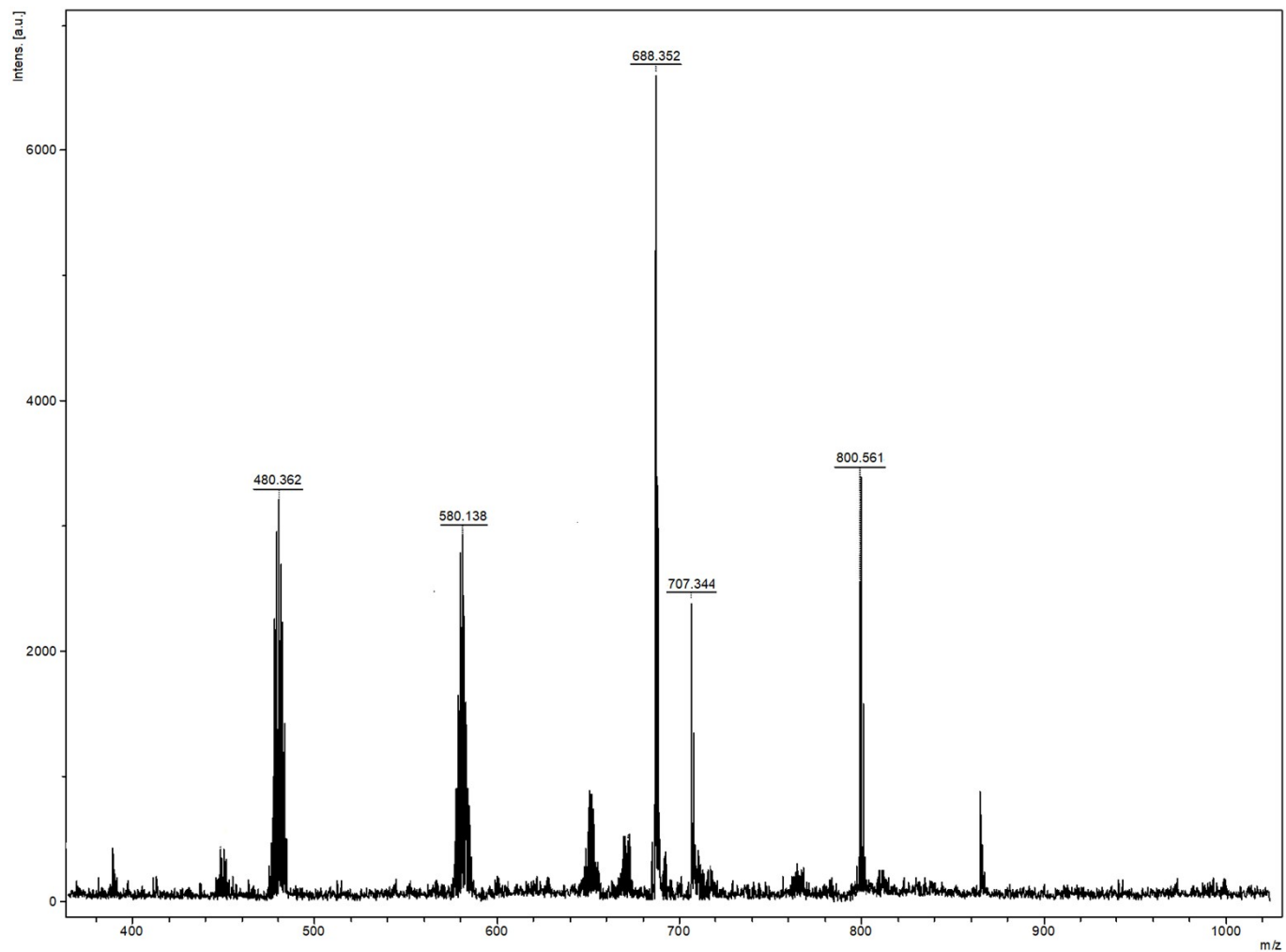


Figure S5. Mass spectrum (MALDI) of compound 4

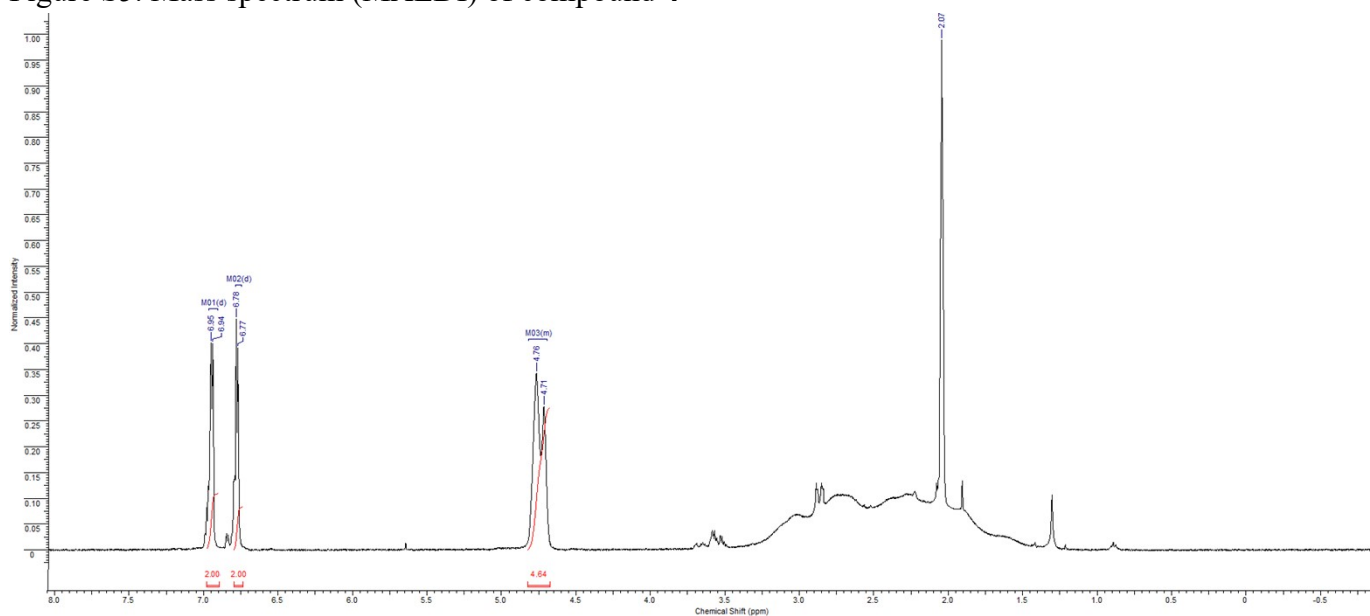


Figure S6.  $^1\text{H}$  NMR (400 MHz,  $(\text{CD}_3)_2\text{CO}$ ) spectrum of compound 5

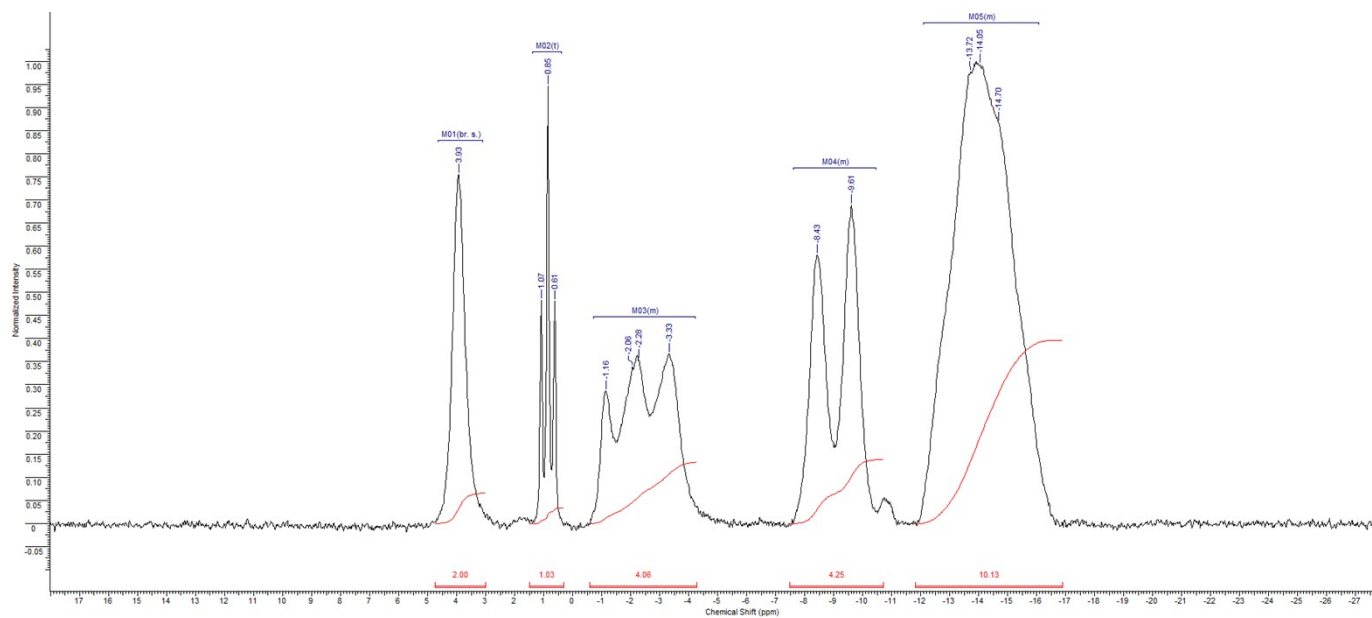


Figure S7.  $^{11}\text{B}$  NMR (128 MHz,  $(\text{CD}_3)_2\text{CO}$ ) spectrum of compound **5**

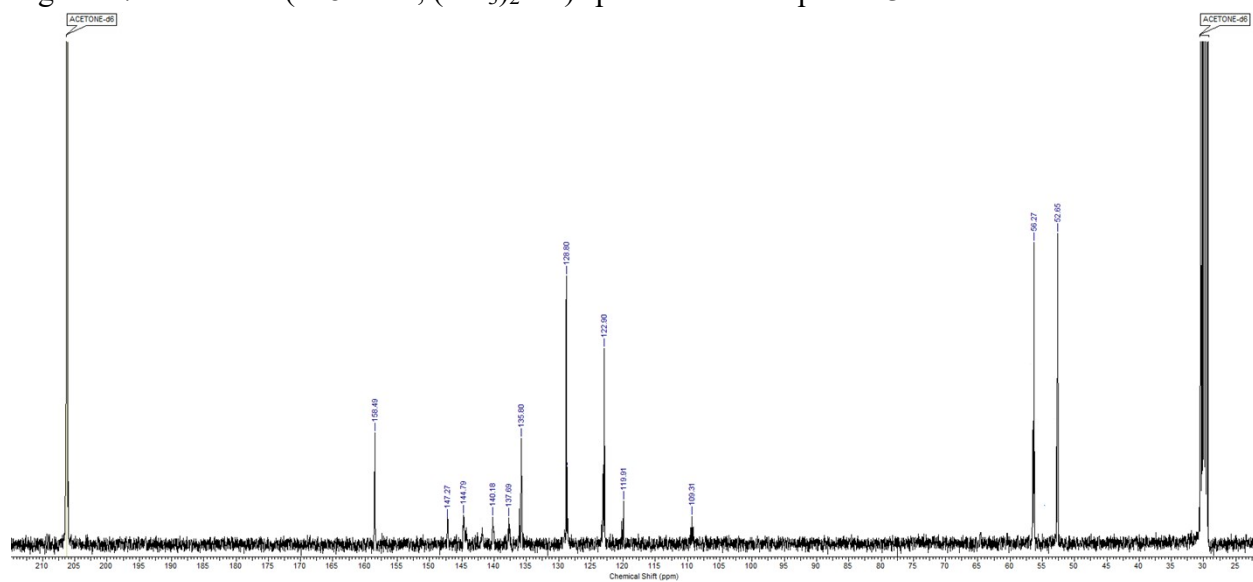


Figure S8.  $^{13}\text{C}$  NMR (100.6 MHz,  $(\text{CD}_3)_2\text{CO}$ ) spectrum of compound **5**

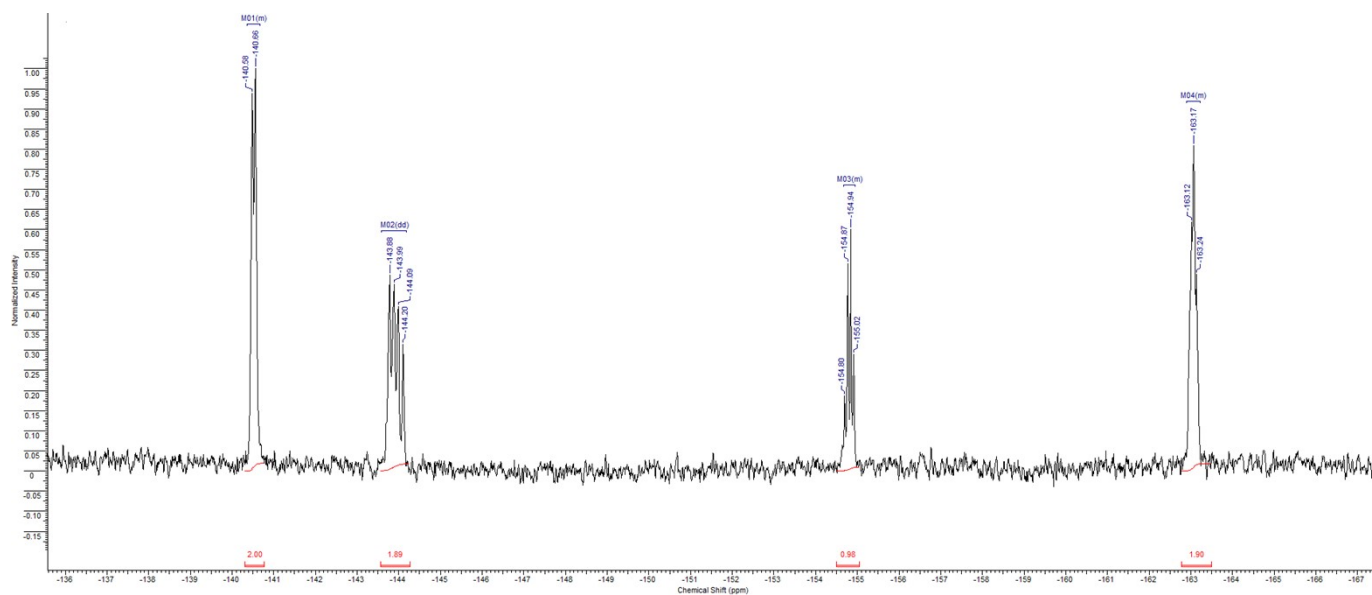


Figure S9.  $^{19}\text{F}$  NMR (282 MHz,  $(\text{CD}_3)_2\text{CO}$ ) spectrum of compound **5**

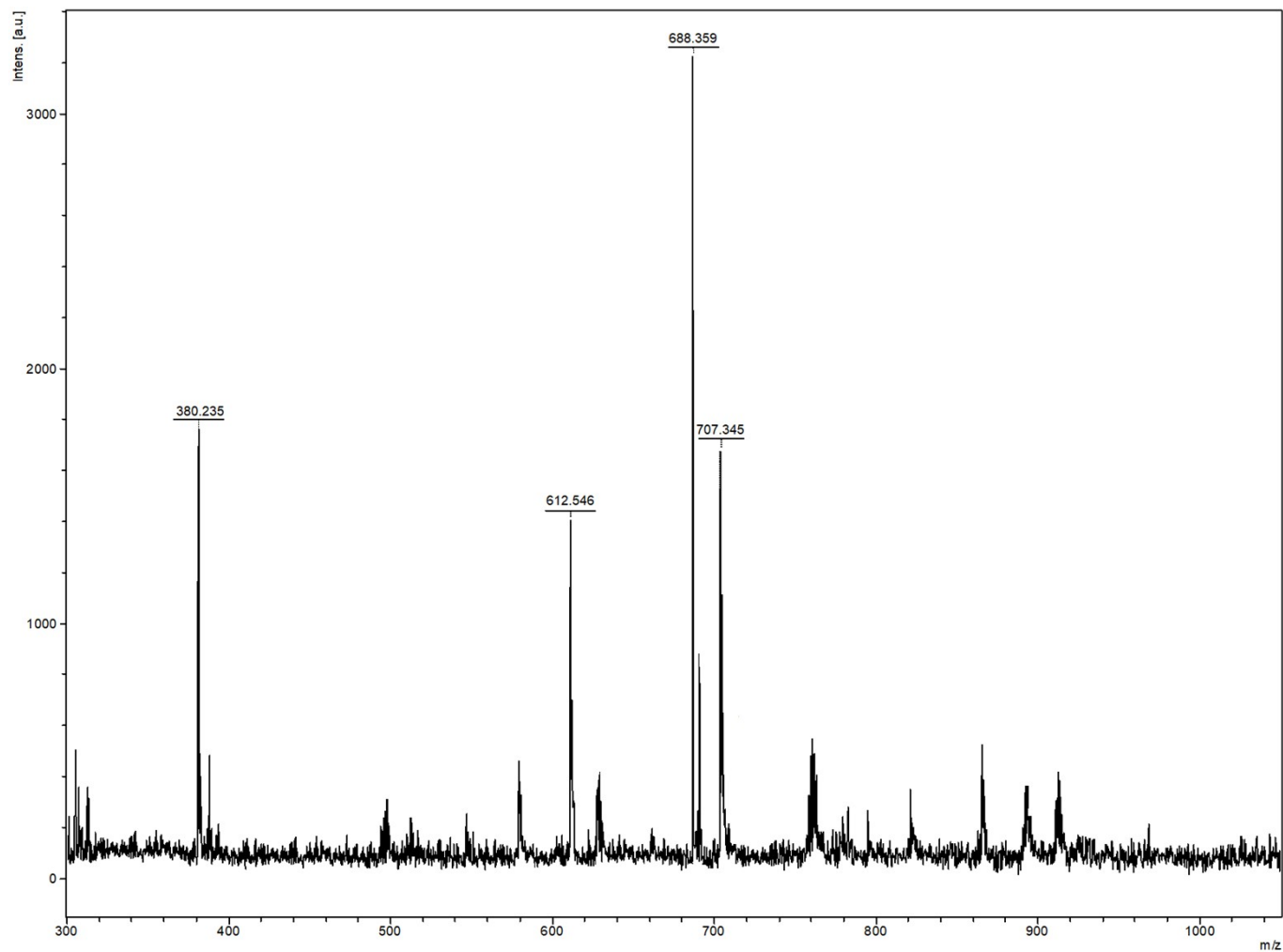


Figure S10. Mass spectrum (MALDI) of compound 5

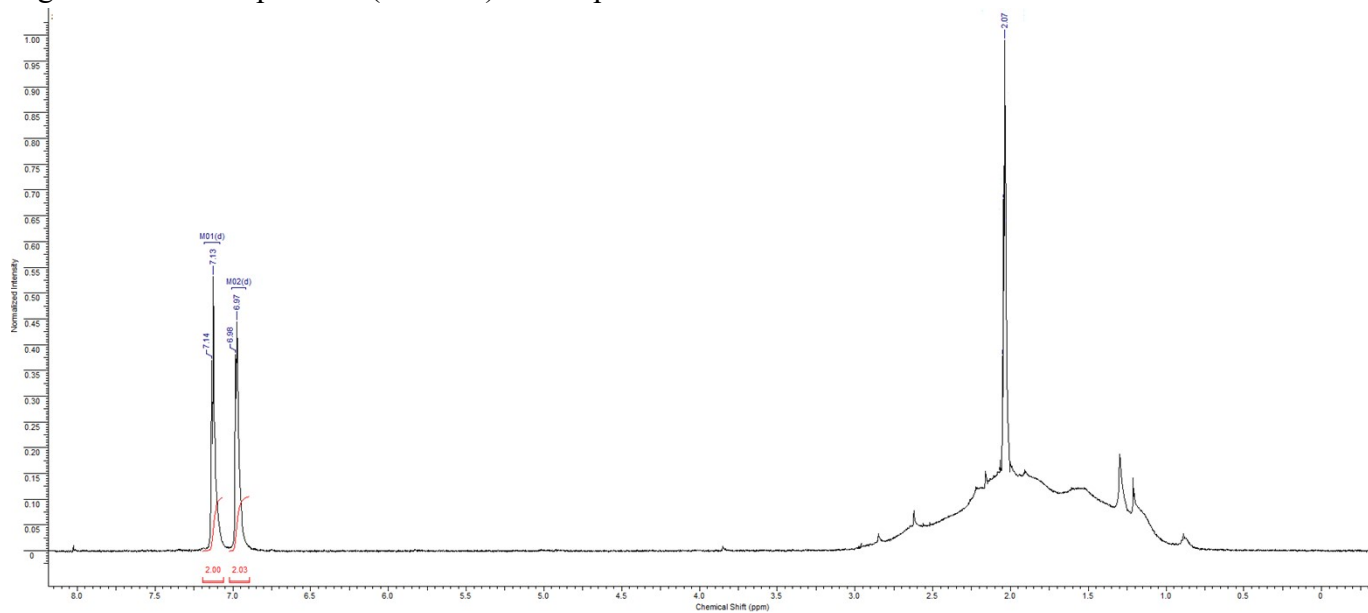


Figure S11. <sup>1</sup>H NMR (400 MHz, (CD<sub>3</sub>)<sub>2</sub>CO) spectrum of compound 7

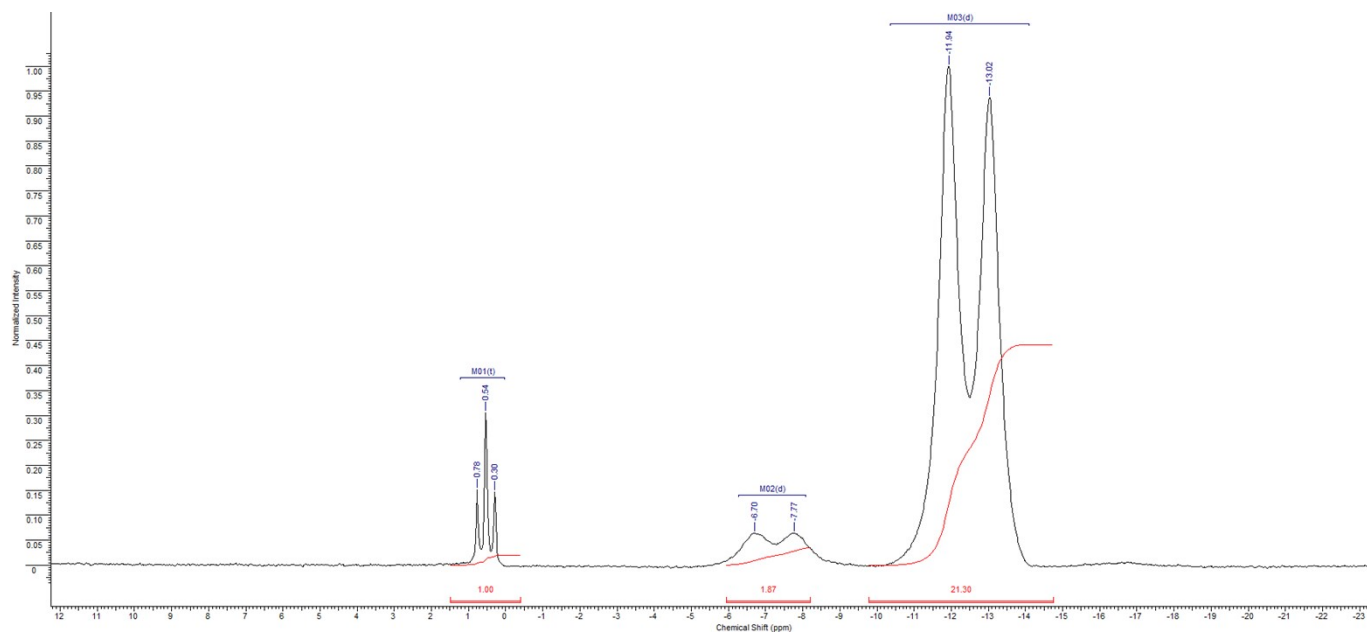


Figure S12.  $^{11}\text{B}$  NMR (128 MHz,  $(\text{CD}_3)_2\text{CO}$ ) spectrum of compound **7**

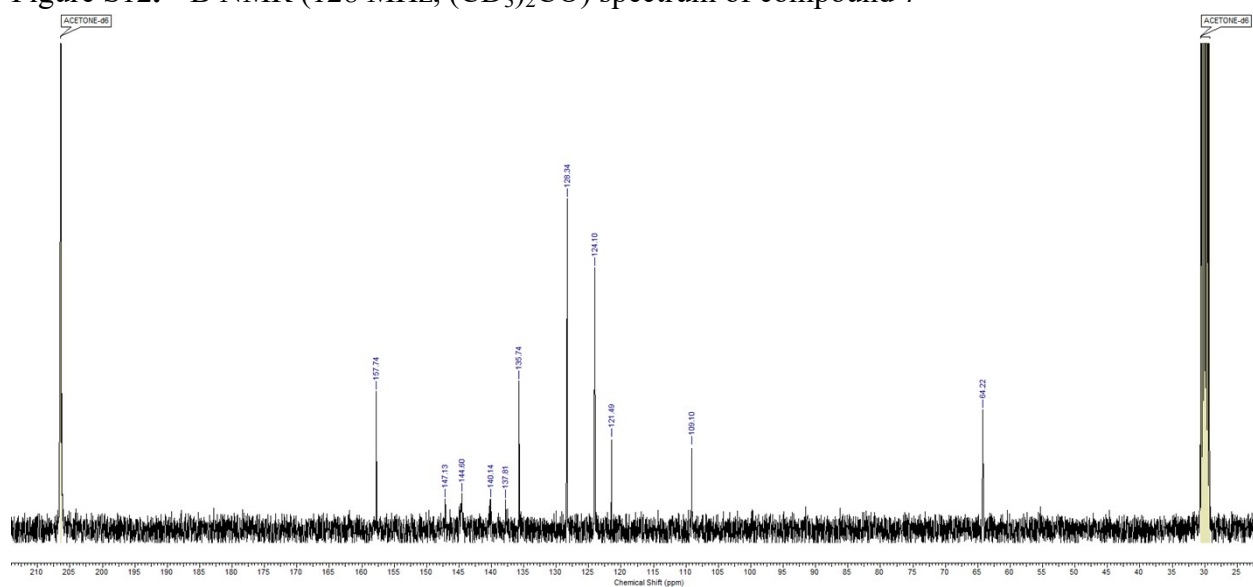


Figure S13.  $^{13}\text{C}$  NMR (100.6 MHz,  $(\text{CD}_3)_2\text{CO}$ ) spectrum of compound **7**

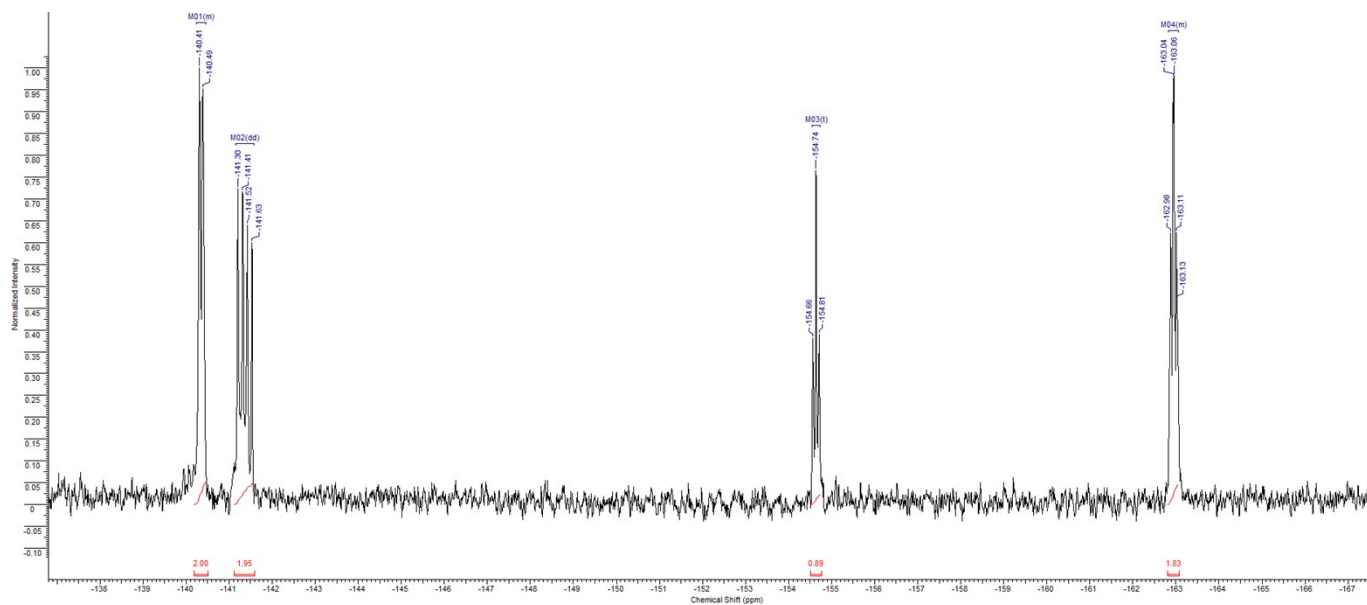


Figure S14.  $^{19}\text{F}$  NMR (282 MHz,  $(\text{CD}_3)_2\text{CO}$ ) spectrum of compound 7

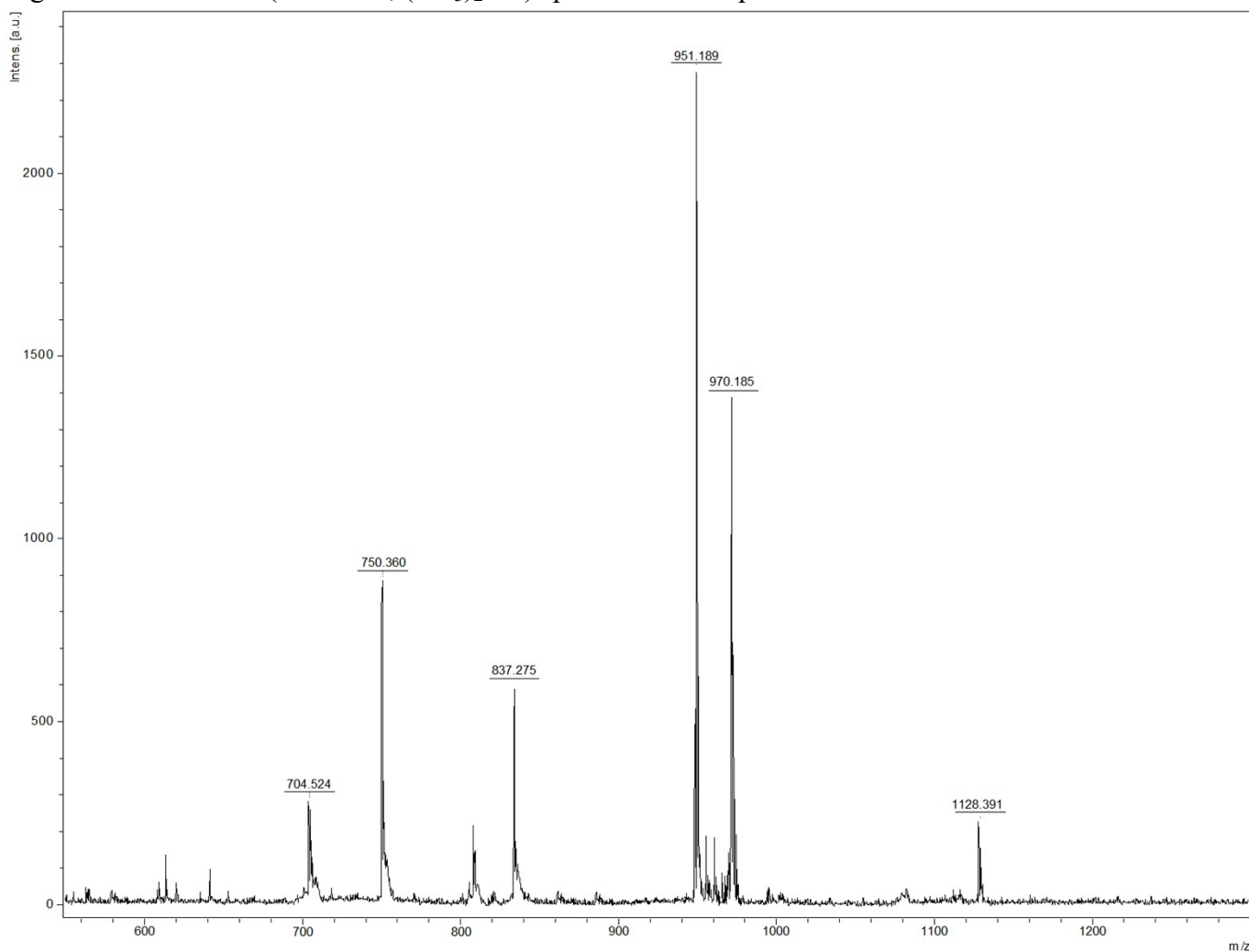


Figure S15. Mass spectrum (MALDI) of compound 7



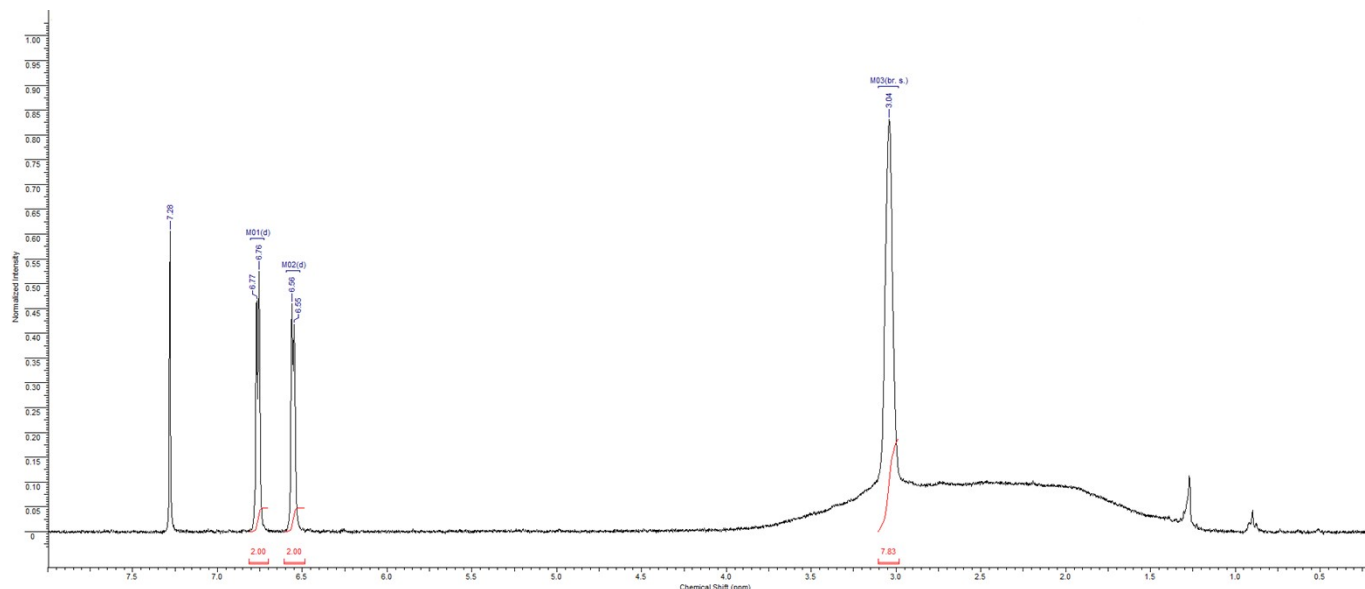


Figure S16.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectrum of compound **8**

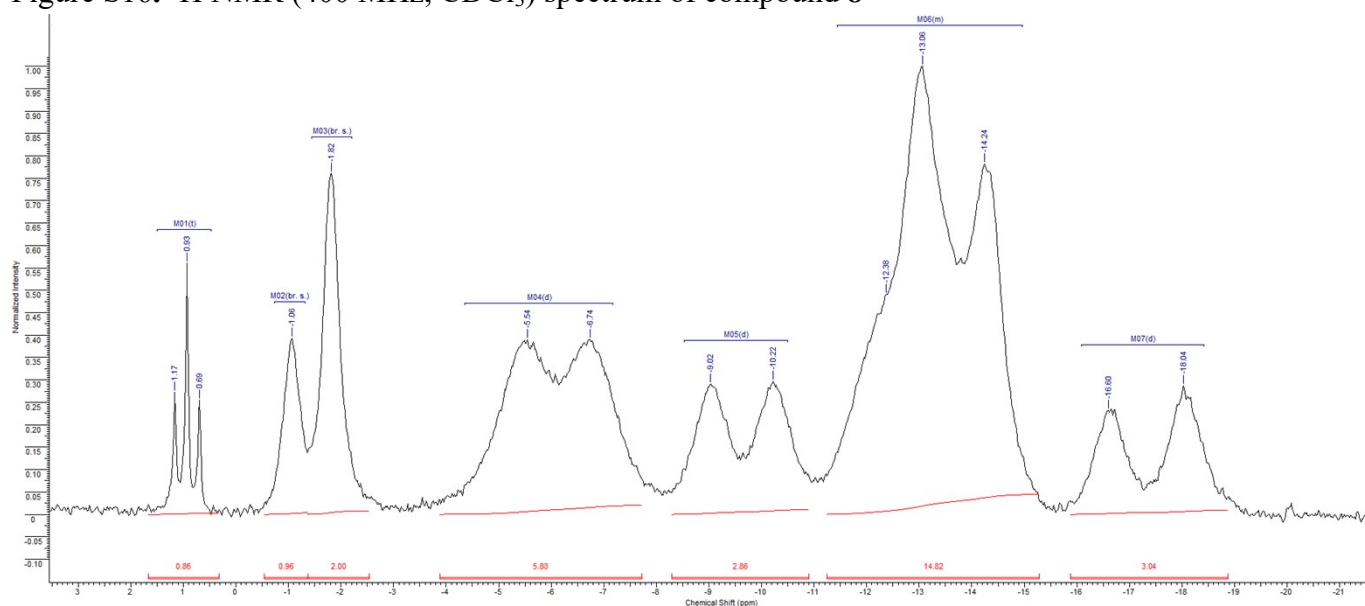


Figure S17.  $^{11}\text{B}$  NMR (128 MHz,  $\text{CDCl}_3$ ) spectrum of compound **8**

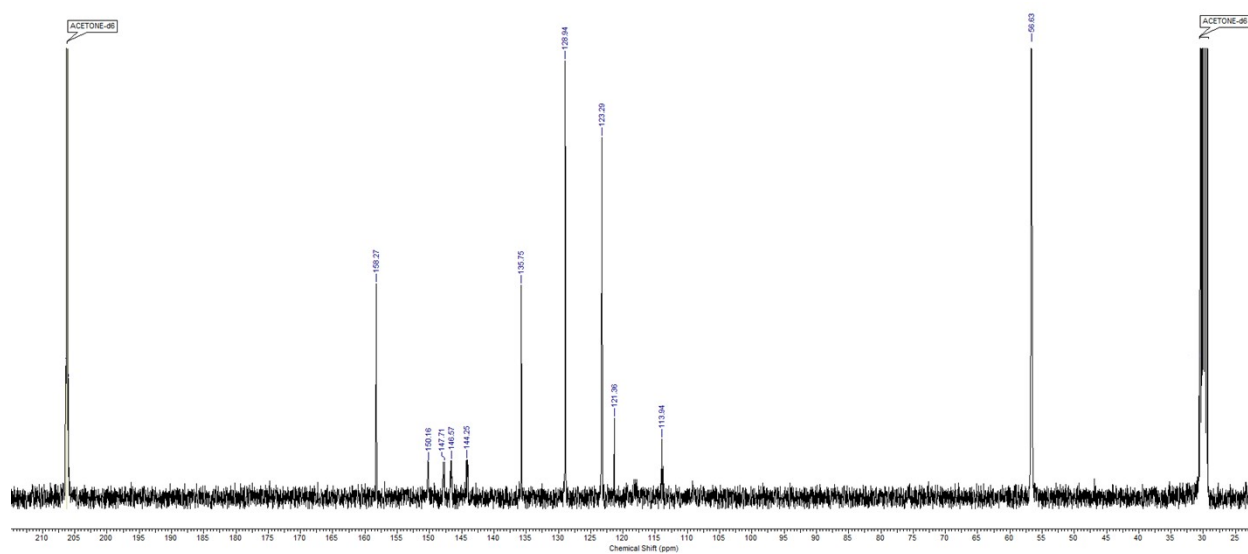


Figure S18.  $^{13}\text{C}$  NMR (100.6 MHz,  $(\text{CD}_3)_2\text{CO}$ ) spectrum of compound **8**

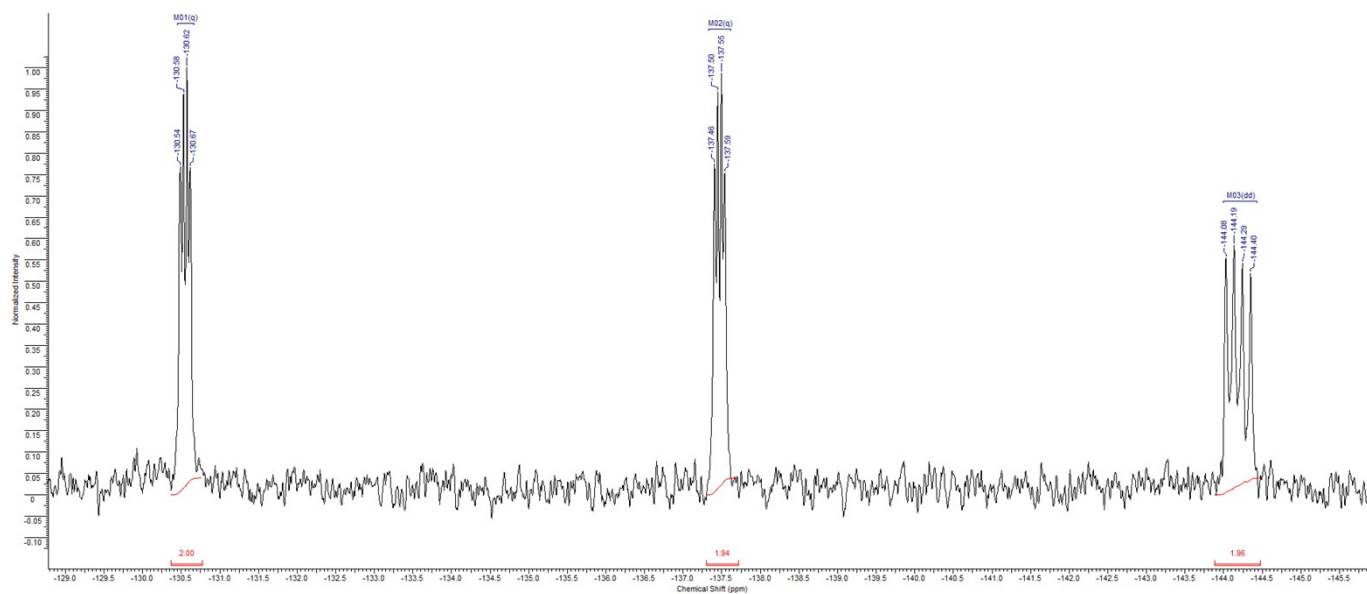


Figure S19.  $^{19}\text{F}$  NMR (282 MHz,  $\text{CDCl}_3$ ) spectrum of compound **8**

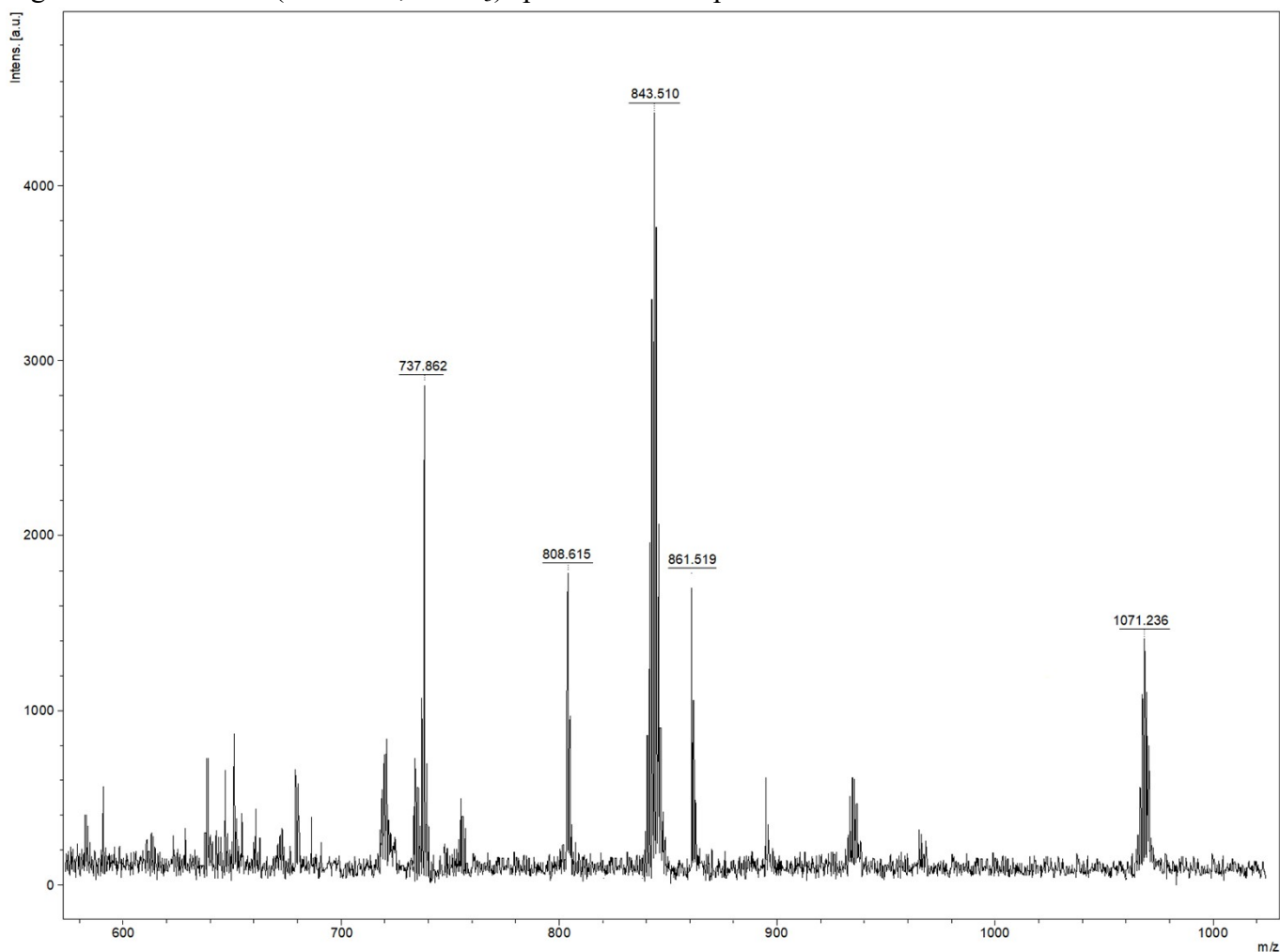


Figure S20. Mass spectrum (MALDI) of compound **8**

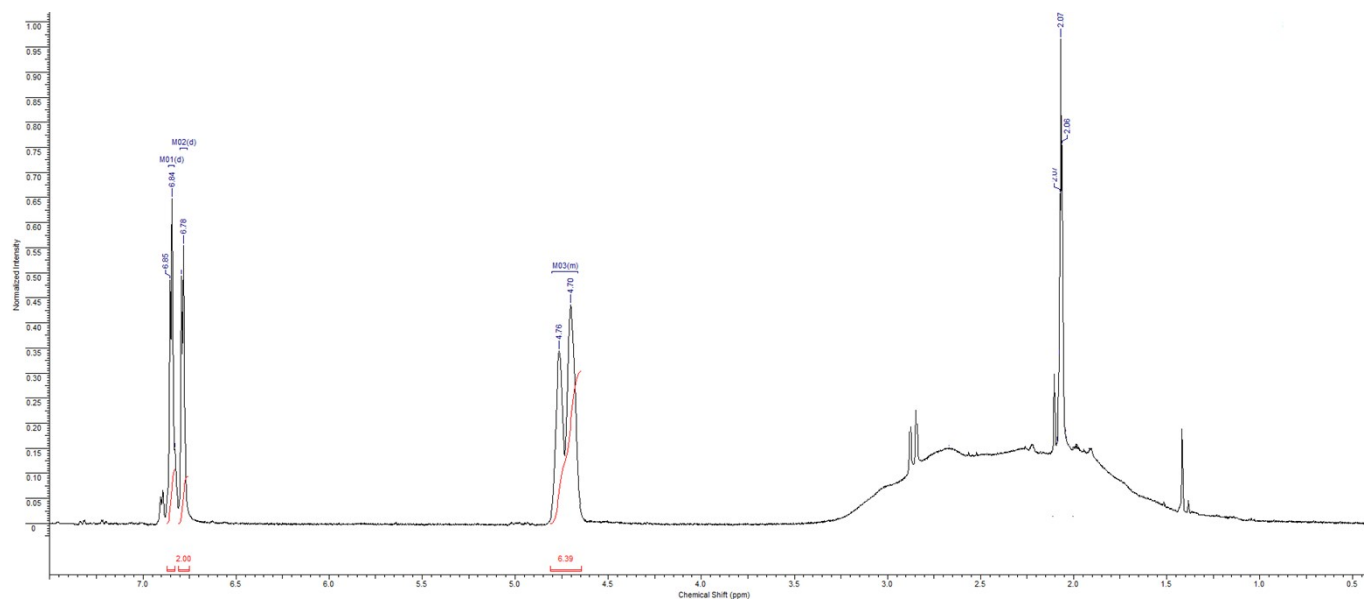


Figure S21.  $^1\text{H}$  NMR (400 MHz,  $(\text{CD}_3)_2\text{CO}$ ) spectrum of compound **9**

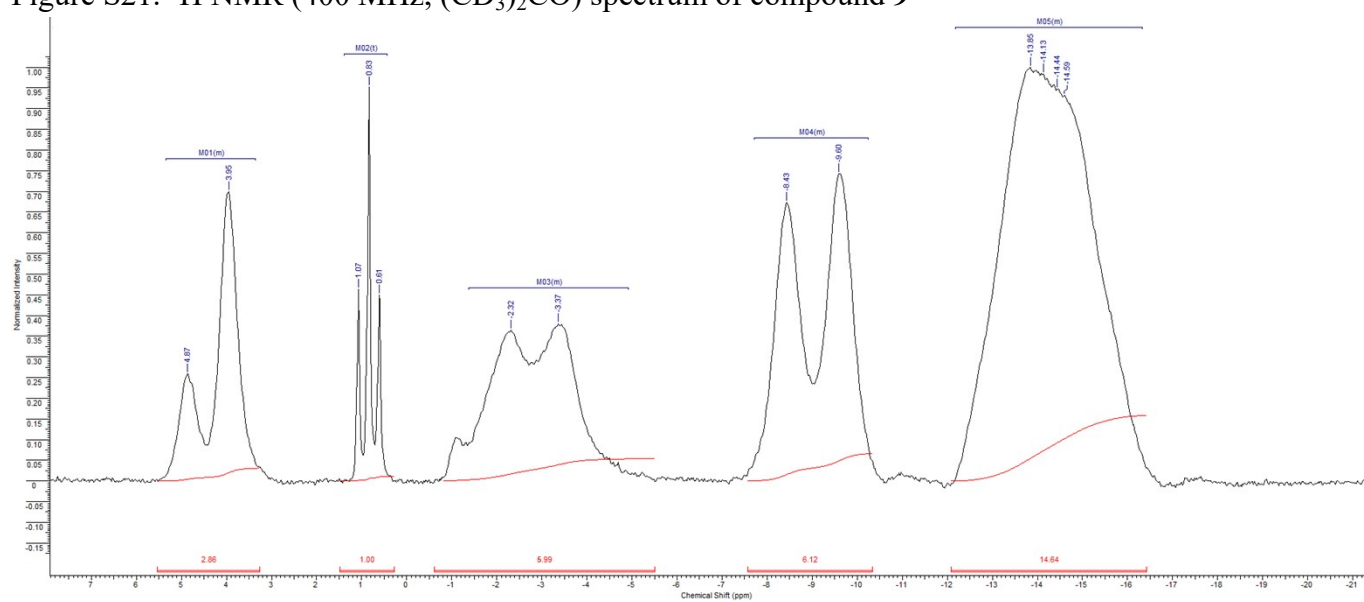


Figure S22.  $^{11}\text{B}$  NMR (128 MHz,  $(\text{CD}_3)_2\text{CO}$ ) spectrum of compound **9**

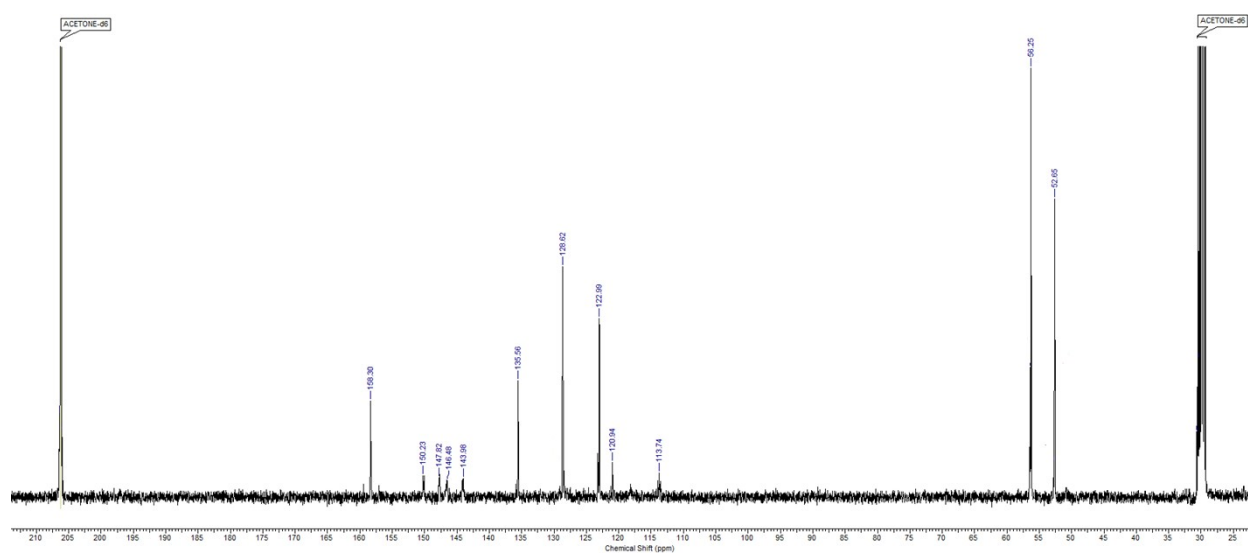


Figure S23.  $^{13}\text{C}$  NMR (100.6 MHz,  $(\text{CD}_3)_2\text{CO}$ ) spectrum of compound **9**

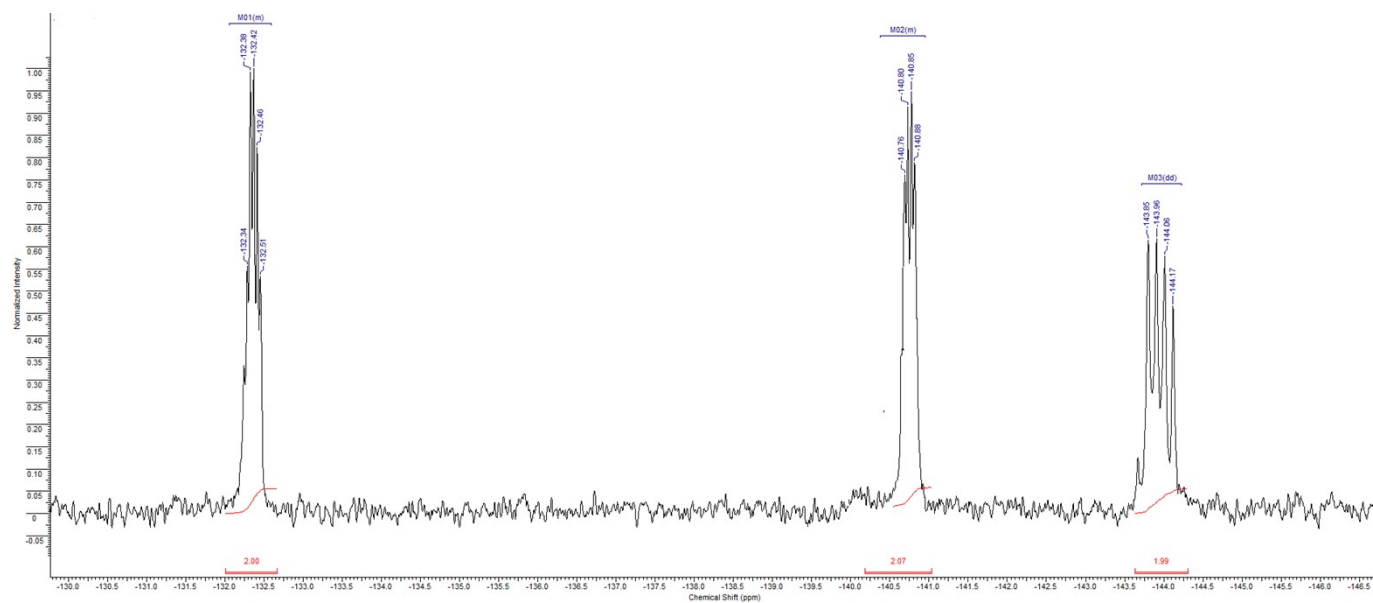


Figure S24.  $^{19}\text{F}$  NMR (282 MHz,  $(\text{CD}_3)_2\text{CO}$ ) spectrum of compound **9**

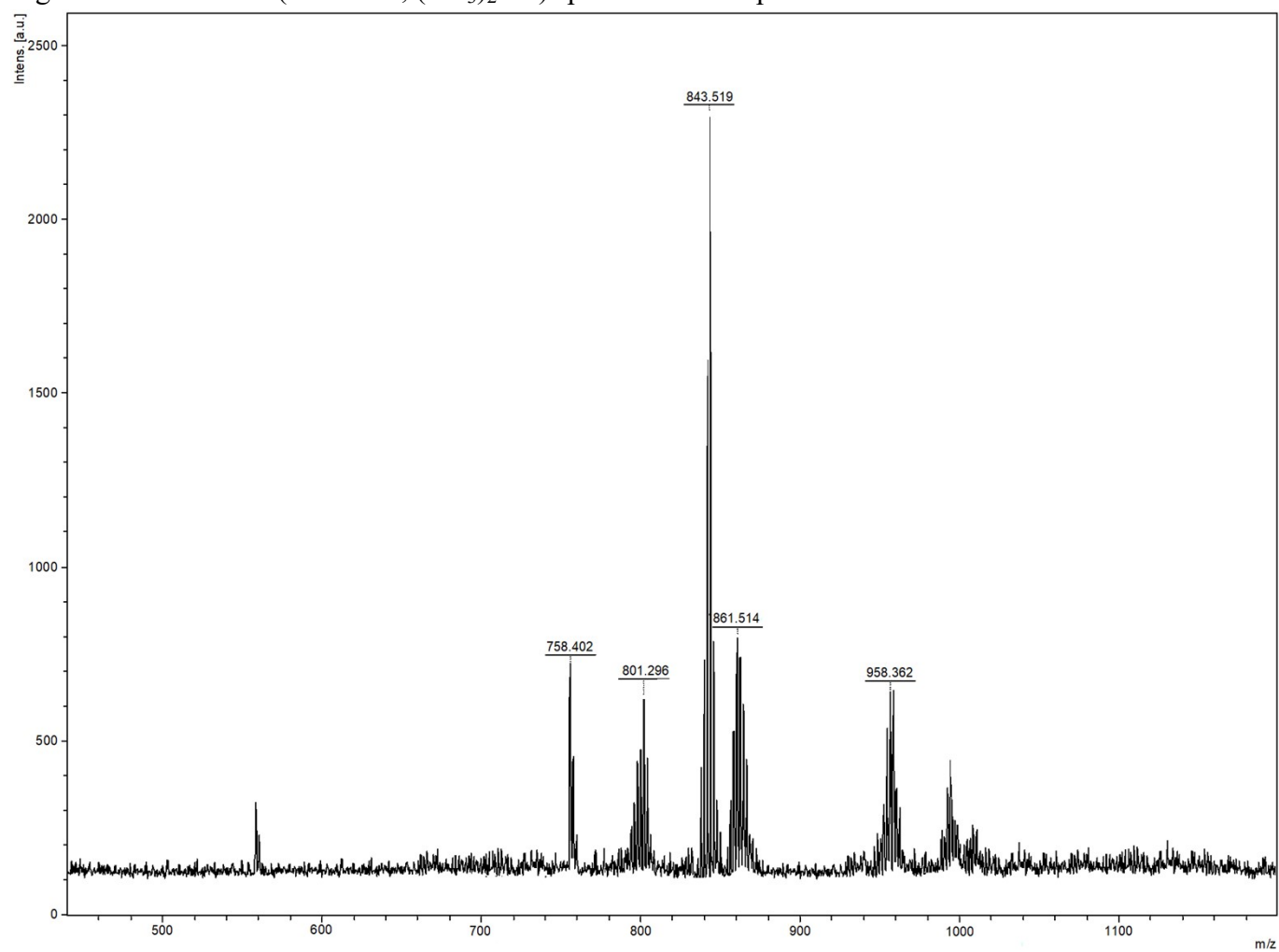


Figure S25. Mass spectrum (MALDI) of compound **9**

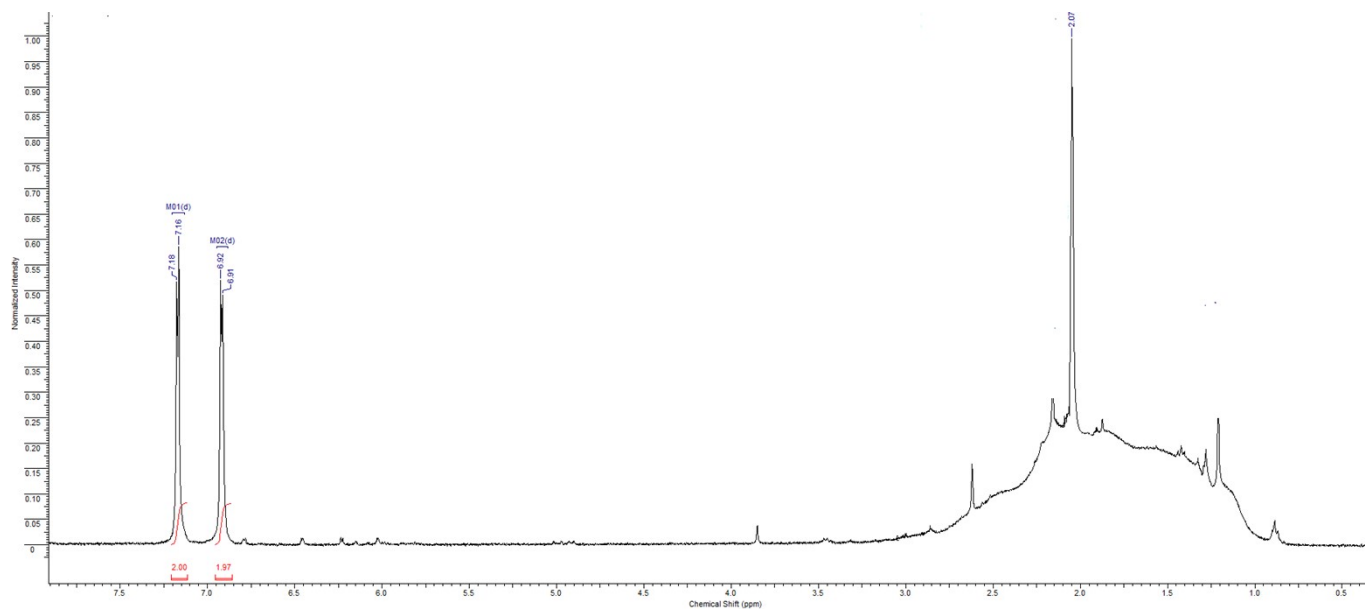


Figure S26.  $^1\text{H}$  NMR (400 MHz,  $(\text{CD}_3)_2\text{CO}$ ) spectrum of compound **10**

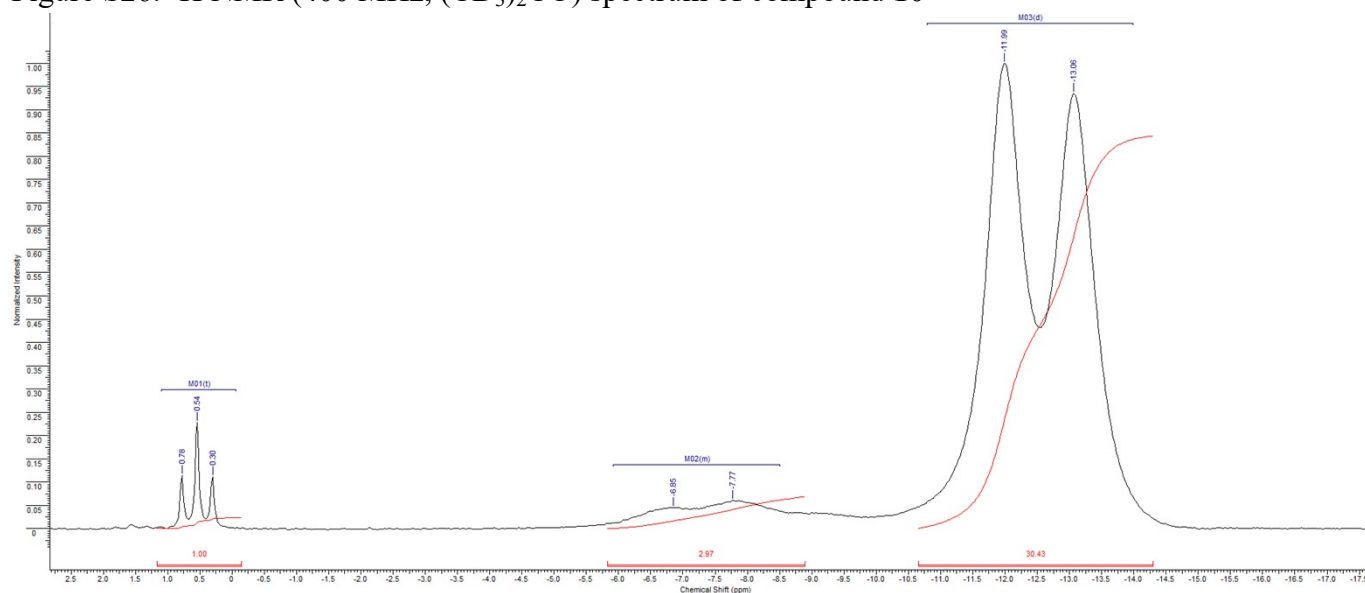


Figure S27.  $^{11}\text{B}$  NMR (128 MHz,  $(\text{CD}_3)_2\text{CO}$ ) spectrum of compound **10**

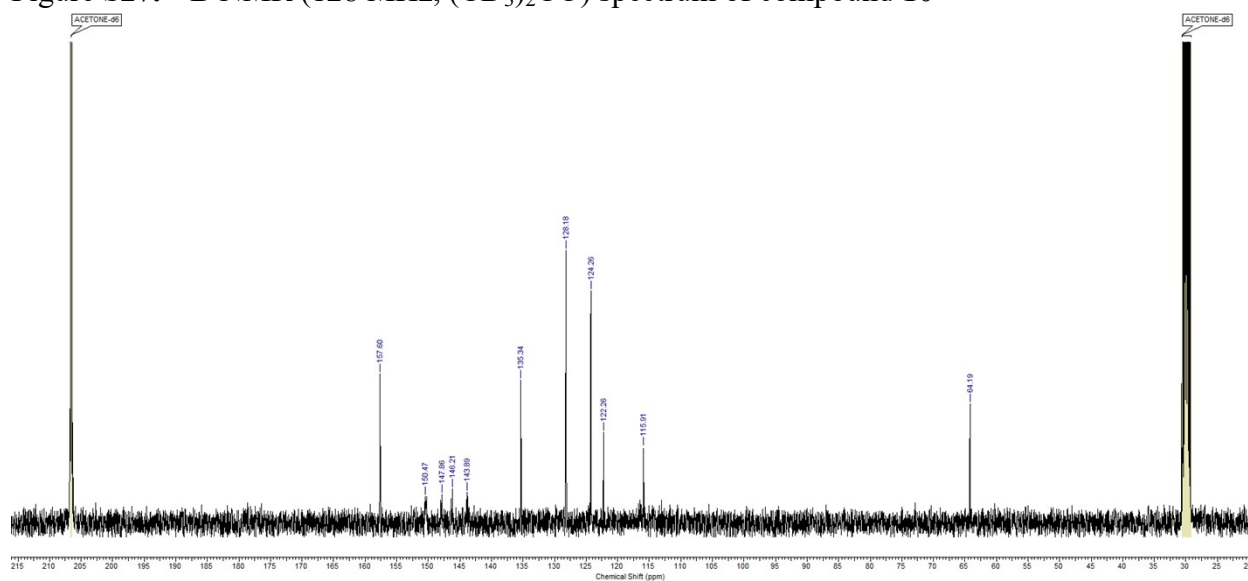


Figure S28.  $^{13}\text{C}$  NMR (100.6 MHz,  $(\text{CD}_3)_2\text{CO}$ ) spectrum of compound **10**

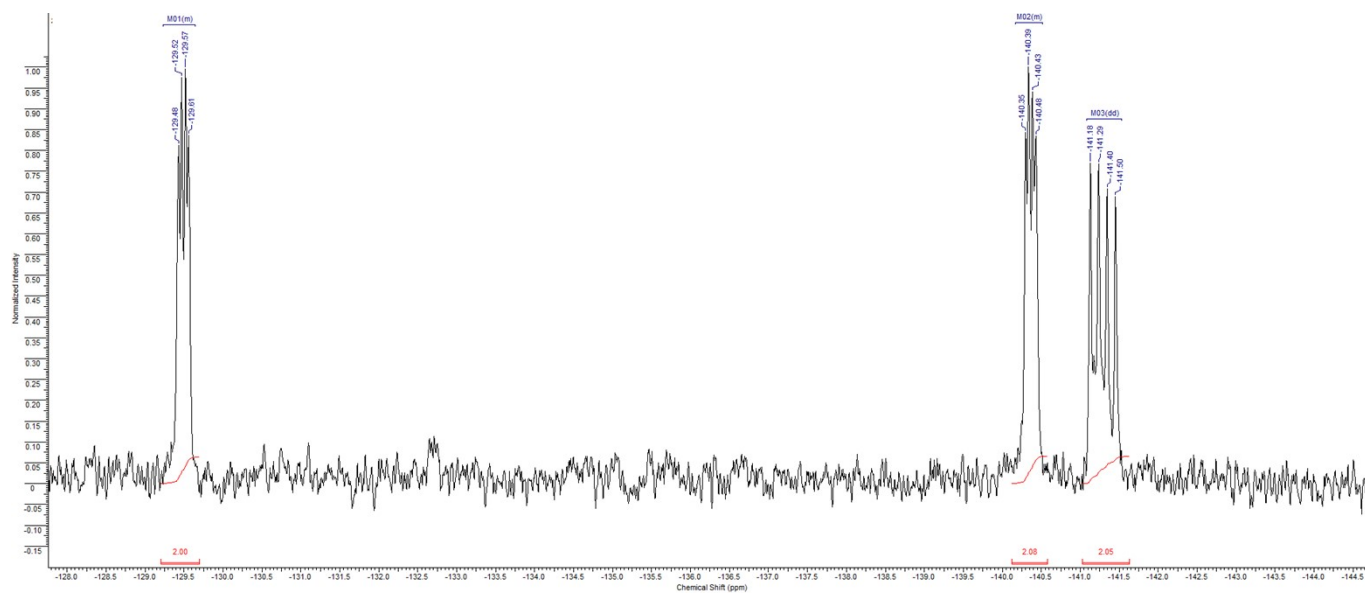


Figure S29.  $^{19}\text{F}$  NMR (282 MHz,  $(\text{CD}_3)_2\text{CO}$ ) spectrum of compound **10**

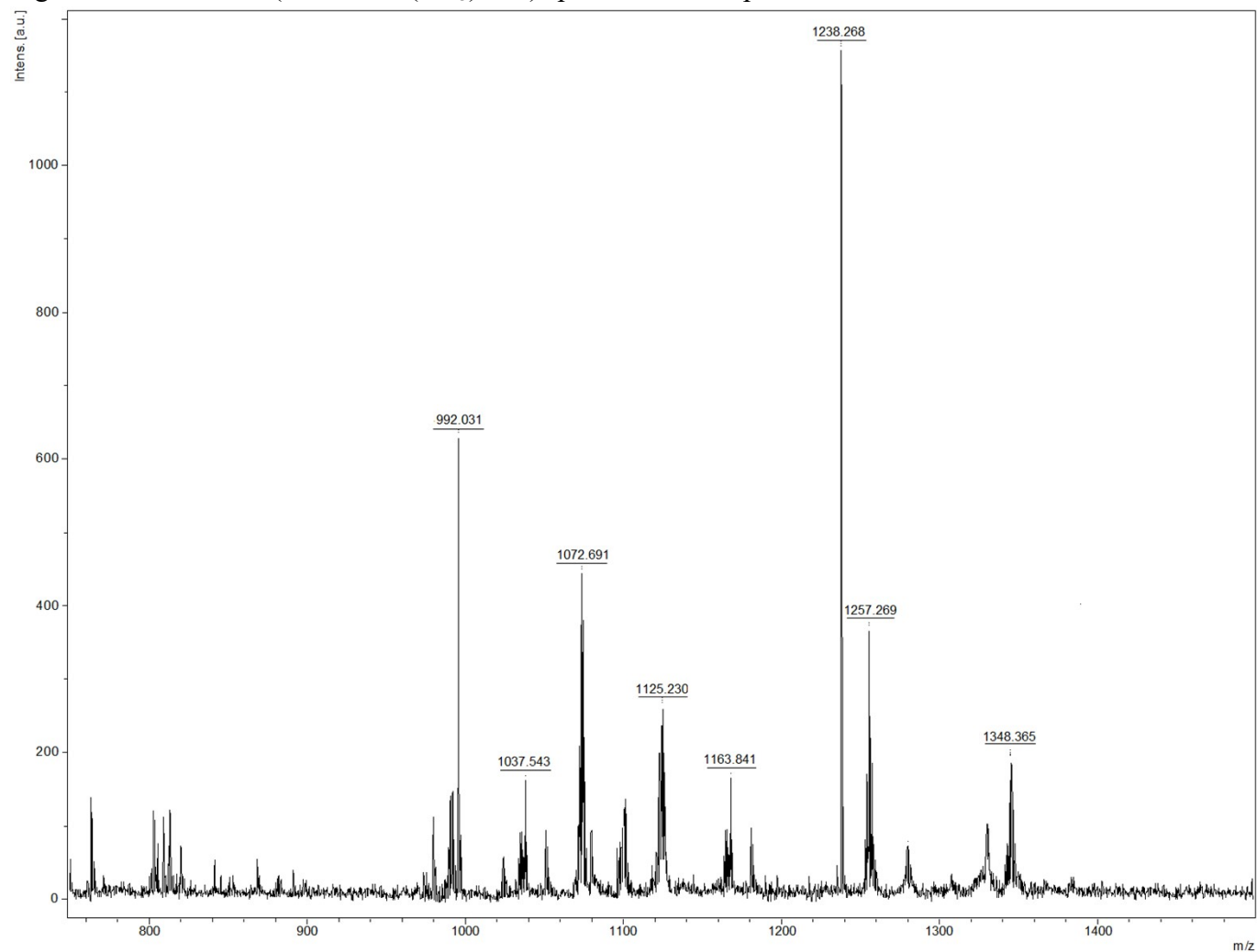


Figure S30. Mass spectrum (MALDI) of compound **10**

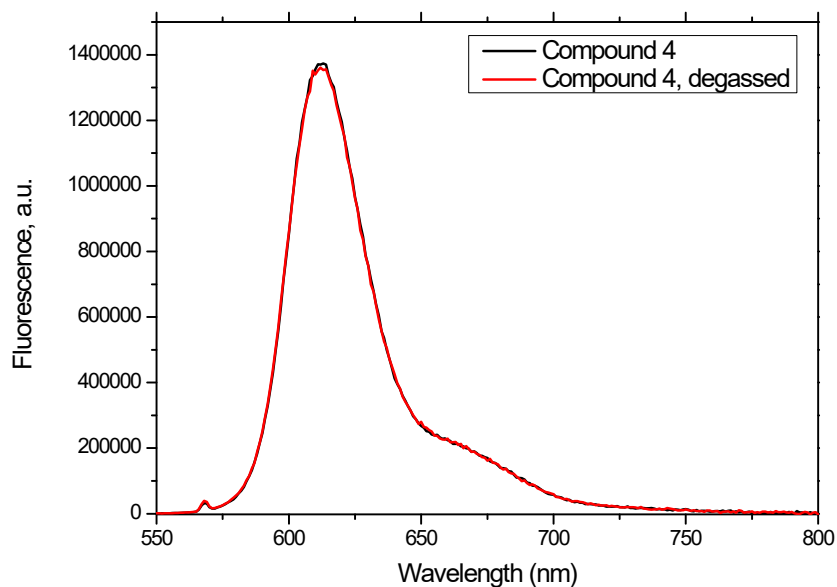


Fig. S31. Fluorescence spectra of compound **4** in air-saturated (black line) and degassed (red line) acetone solutions. Degassing of solutions in acetone was carried out by the freeze-pump-thaw method (3 cycles). Excitation at 567 nm.

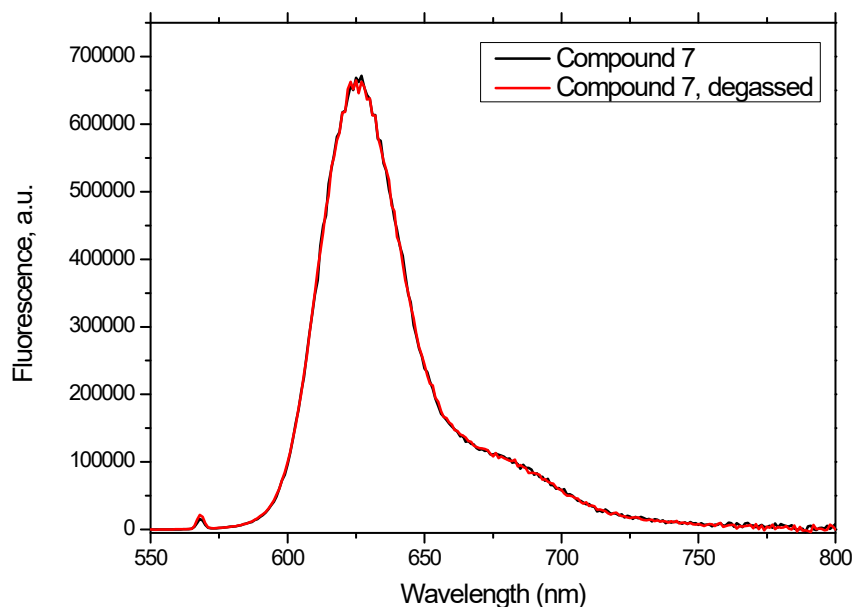


Fig. S32. Fluorescence spectra of compound **7** in air-saturated (black line) and degassed (red line) acetone solutions. Degassing of solutions in acetone was carried out by the freeze-pump-thaw method (3 cycles). Excitation at 567 nm.

Table. S1 Comparison of the experimental and theoretical interatomic distances for molecule **4**, **8**.

Bond type	Compound <b>4</b>		Compound <b>8</b>	
	Experiment, Å	Calculations, Å	Experiment, Å	Calculations, Å
C-N	1.36-1.39	1.34-1.38	1.36-1.40	1.34-1.39
B-N	1.56-1.58	1.58	1.57	1.58
B-F	1.38	1.38	1.36-1.38	1.37-1.38
C-S	1.73	1.76	1.75	1.76
B-S	1.86	1.88	1.87	1.88
C-F	1.33	1.33	1.33-1.35	1.33
B-B (carborane)	1.69-1.78	1.76-1.78	1.69-1.77	1.76-1.78
C-B (carborane)	1.69-1.72	1.69-1.71	1.68-1.78	1.69-1.70
C-H (carborane)	1.10	1.08	1.12	1.08