Electronic Supplementary Information

for

Synthesis, structure, photophysical, electrochemical properties and antibacterial activity of brominated BODIPYs

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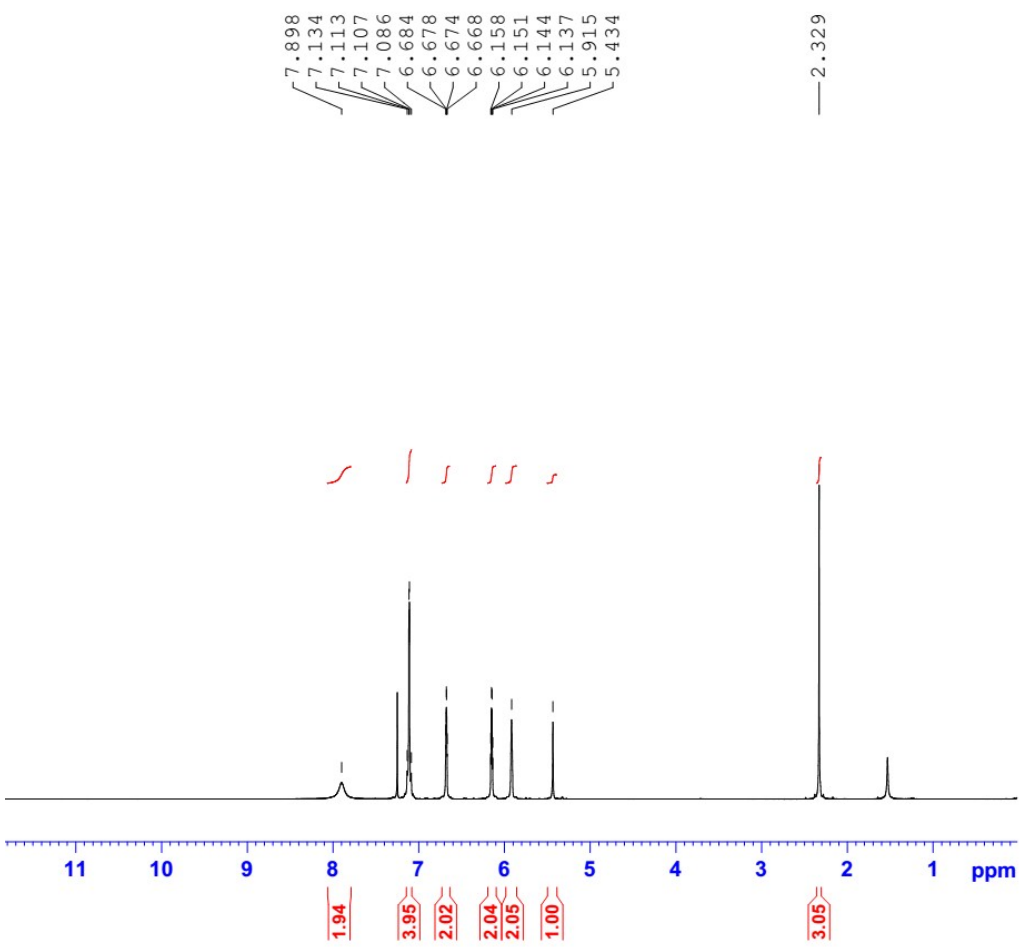

Figure S1. ^{1}H NMR spectrum of 5-(4-Methylphenyl) dipyrromethane.

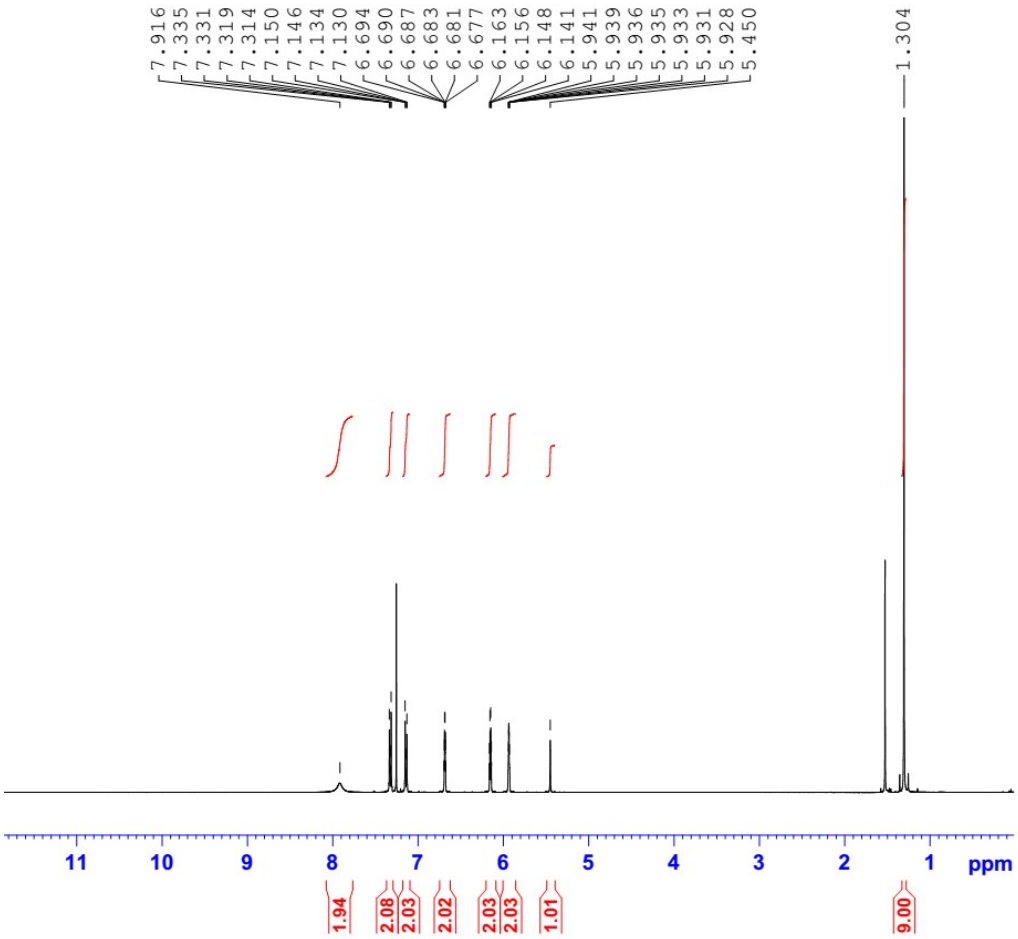

Figure S2.[1]H NMR spectrum of 5-(4-*tert*-Butylphenyl) dipyrromethane.

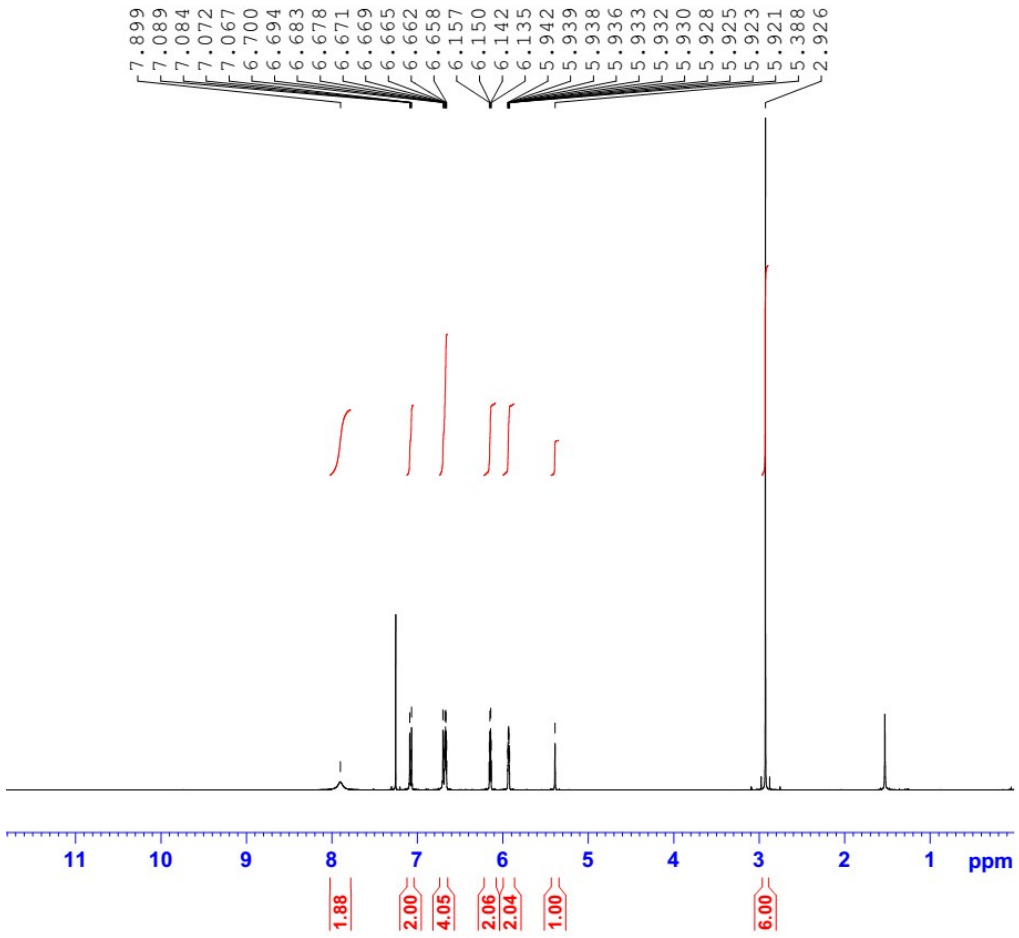

Figure S3. ^{1}H NMR spectrum of 5-(4-N,N'-Dimethylaminophenyl) dipyrromethane.

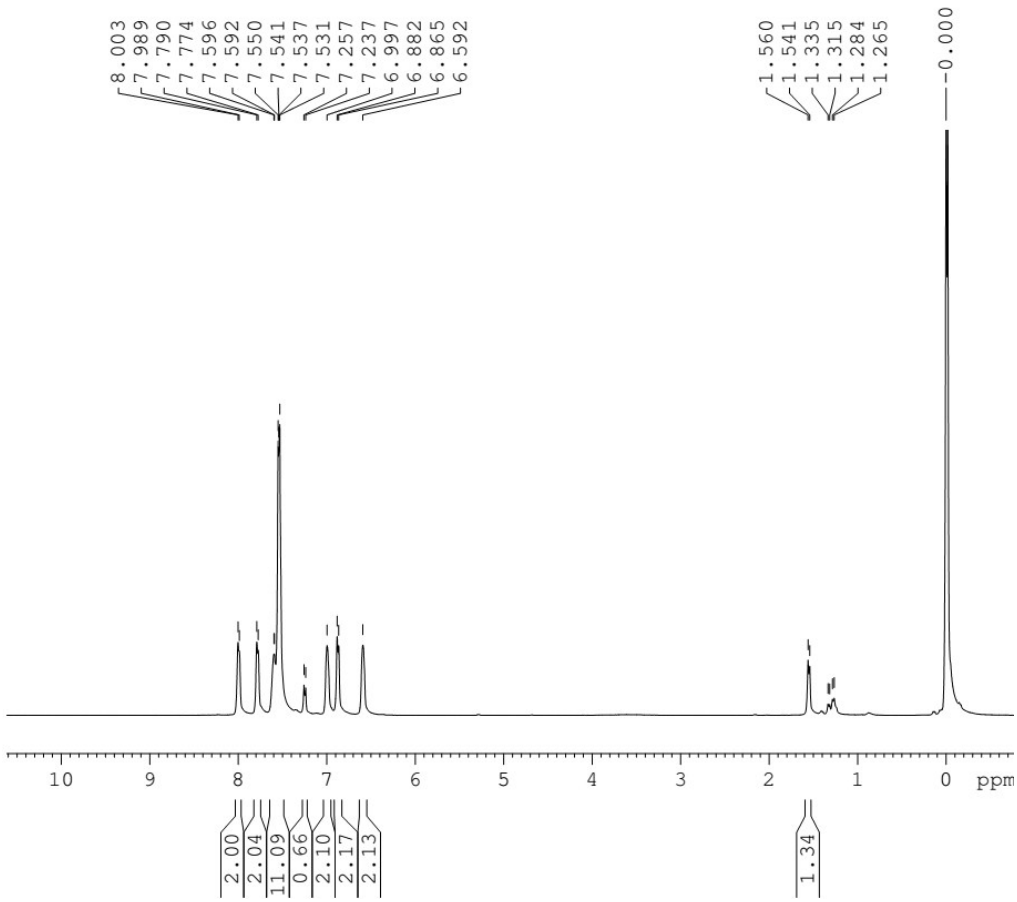

Figure S4. ^{1}H NMR spectrum of compound, **1a**.

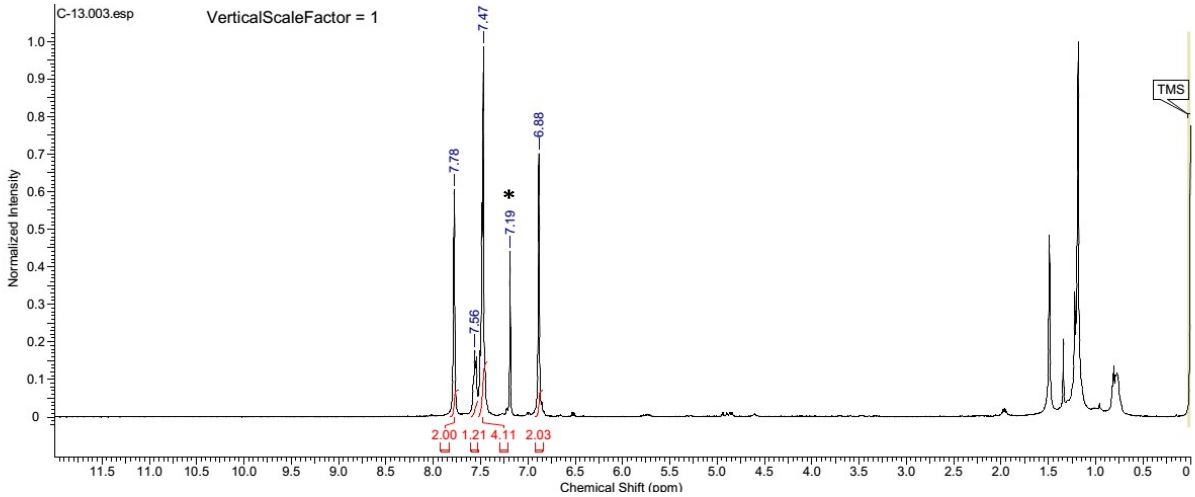

Figure S5. ^{1}H NMR spectrum of compound, **1b**.

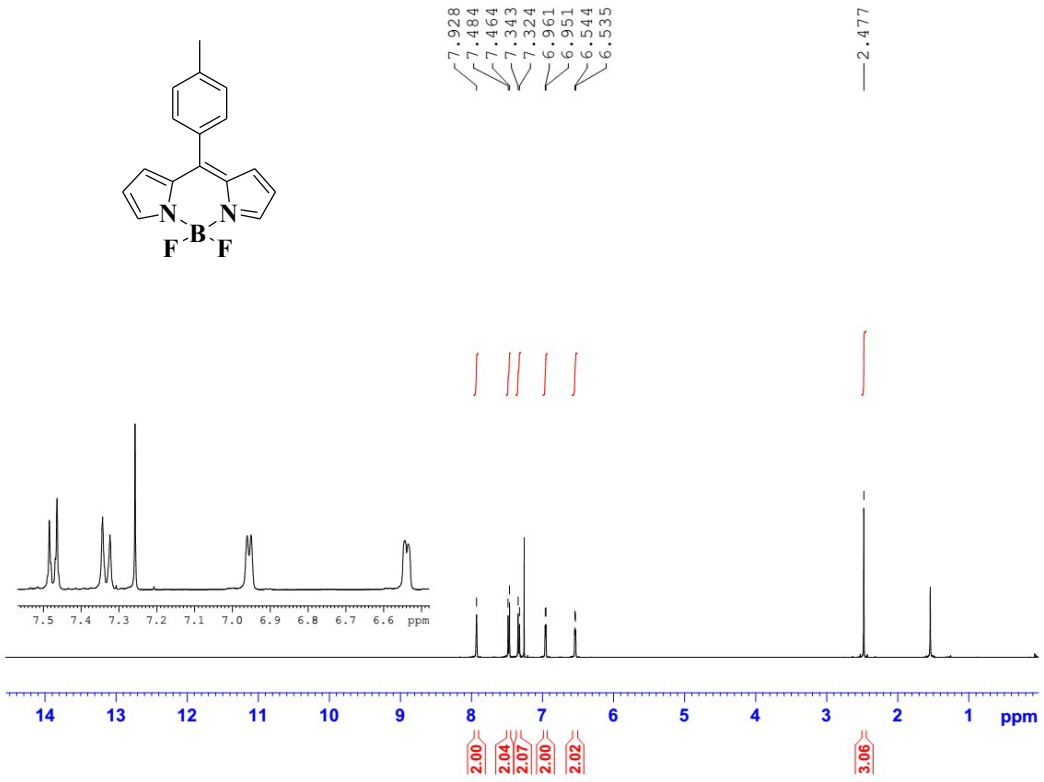

Figure S6. ^{1}H NMR spectrum of compound, **2**.

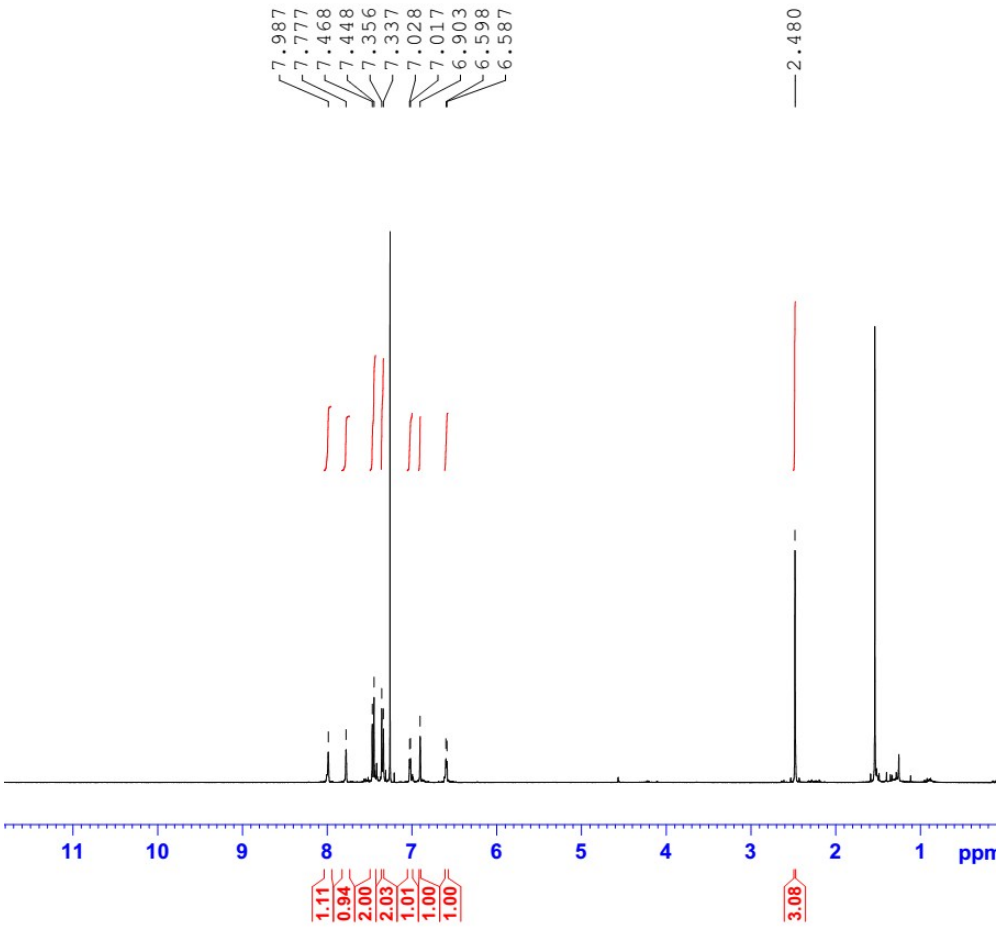

Figure S7. ^{1}H NMR spectrum of compound, **2a**.

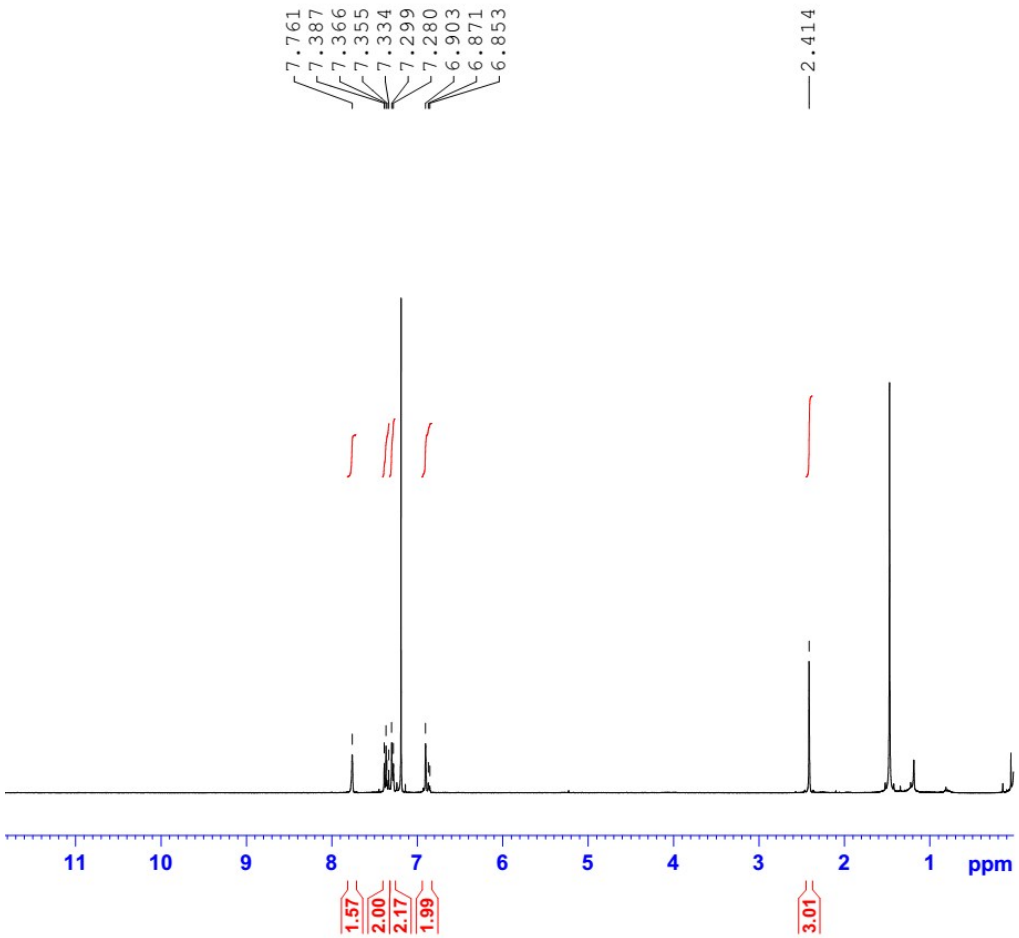

Figure S8. ^{1}H NMR spectrum of compound, **2b**.

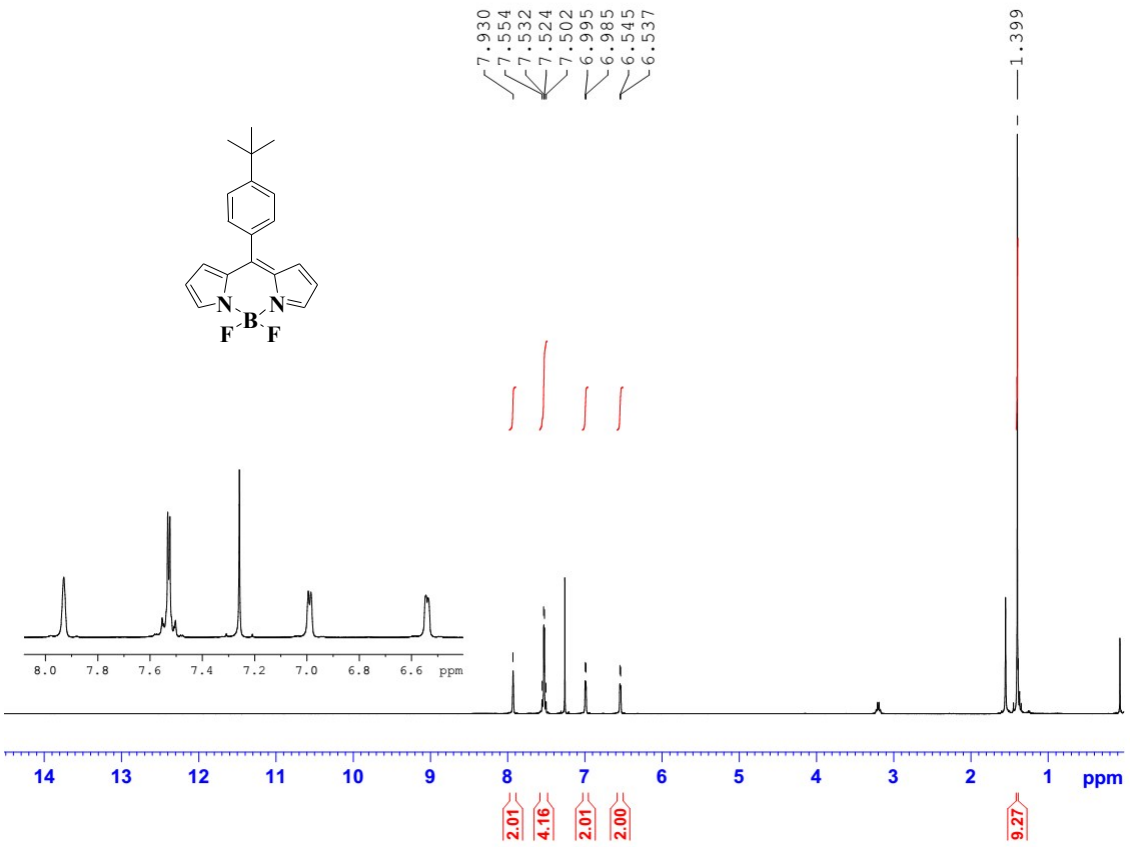

Figure S9. ^{1}H NMR spectrum of compound, **3**.

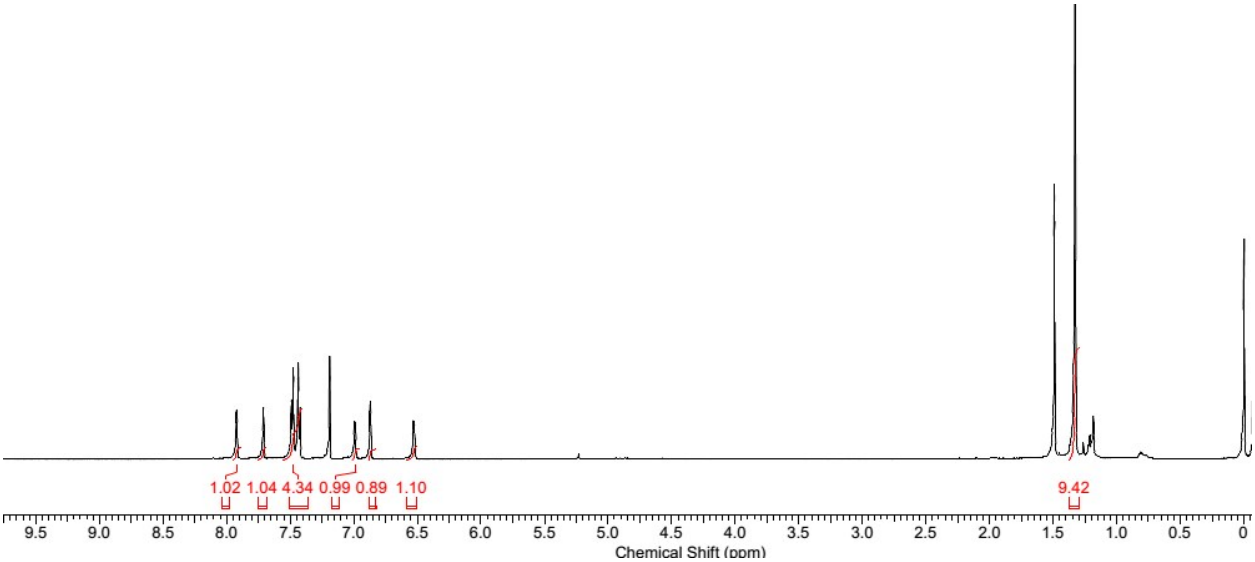

Figure S10. ^{1}H NMR spectrum of compound, **3a**.

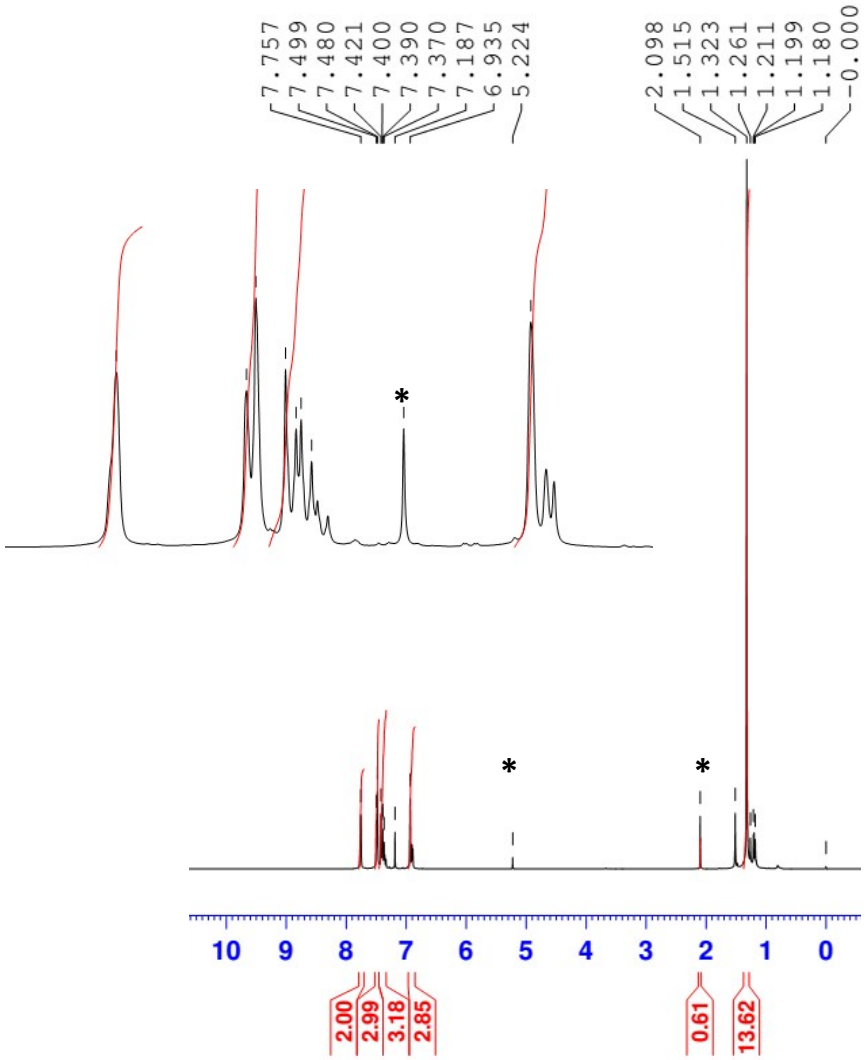

Figure S11. ^{1}H NMR spectrum of compound, **3b**.

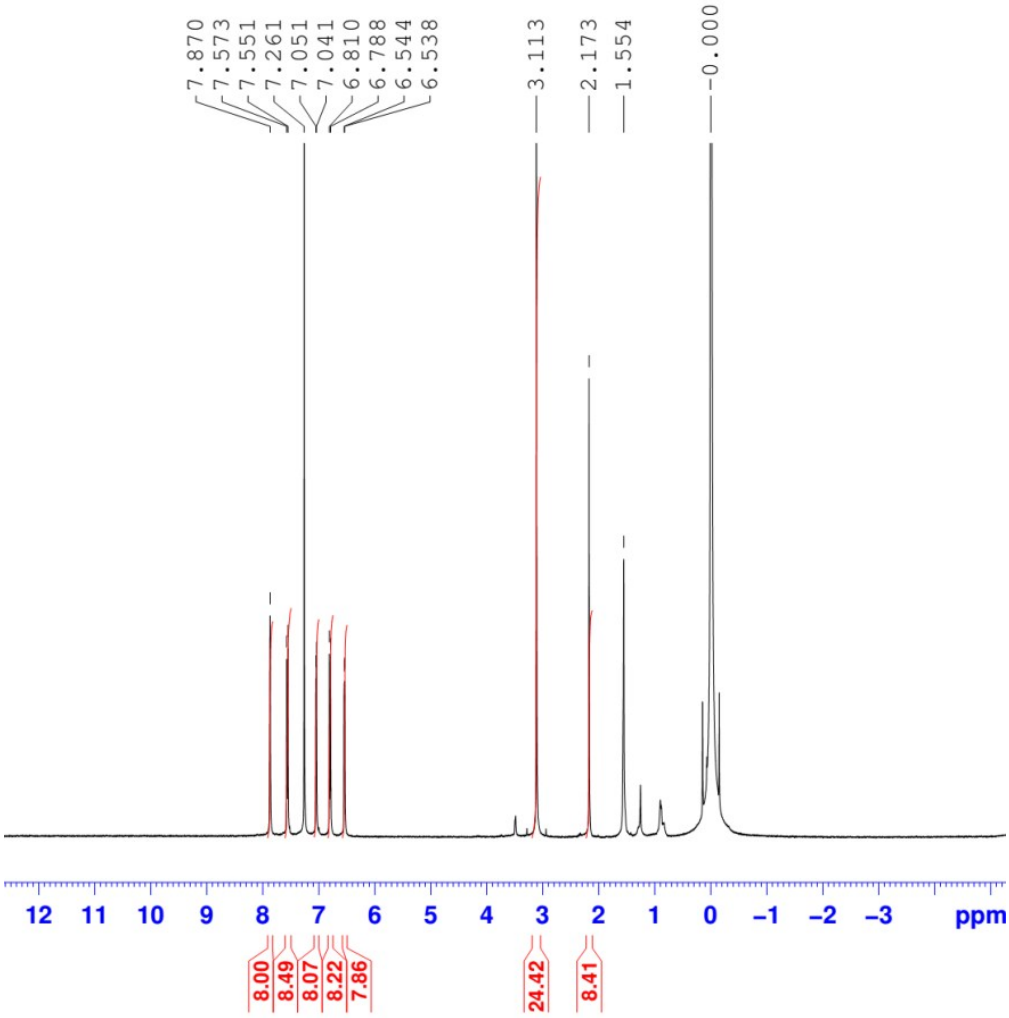

Figure S12. ^{1}H NMR spectrum of compound, **4**.

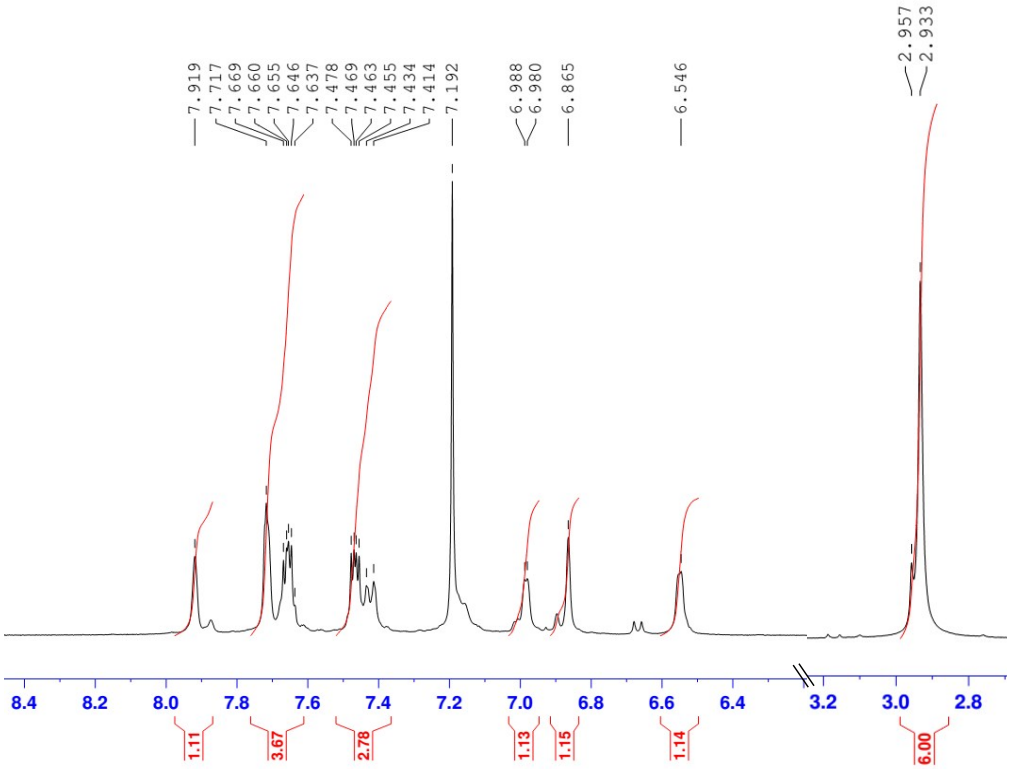

Figure S13. ^{1}H NMR spectrum of compound, **4a**.

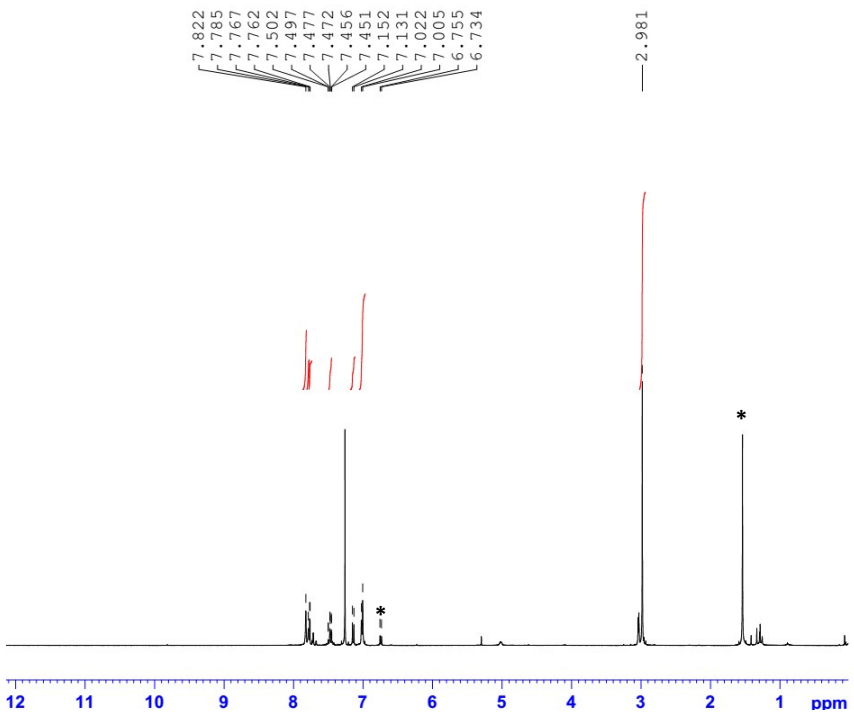

Figure S14. ^{1}H NMR spectrum of compound, **4b**.

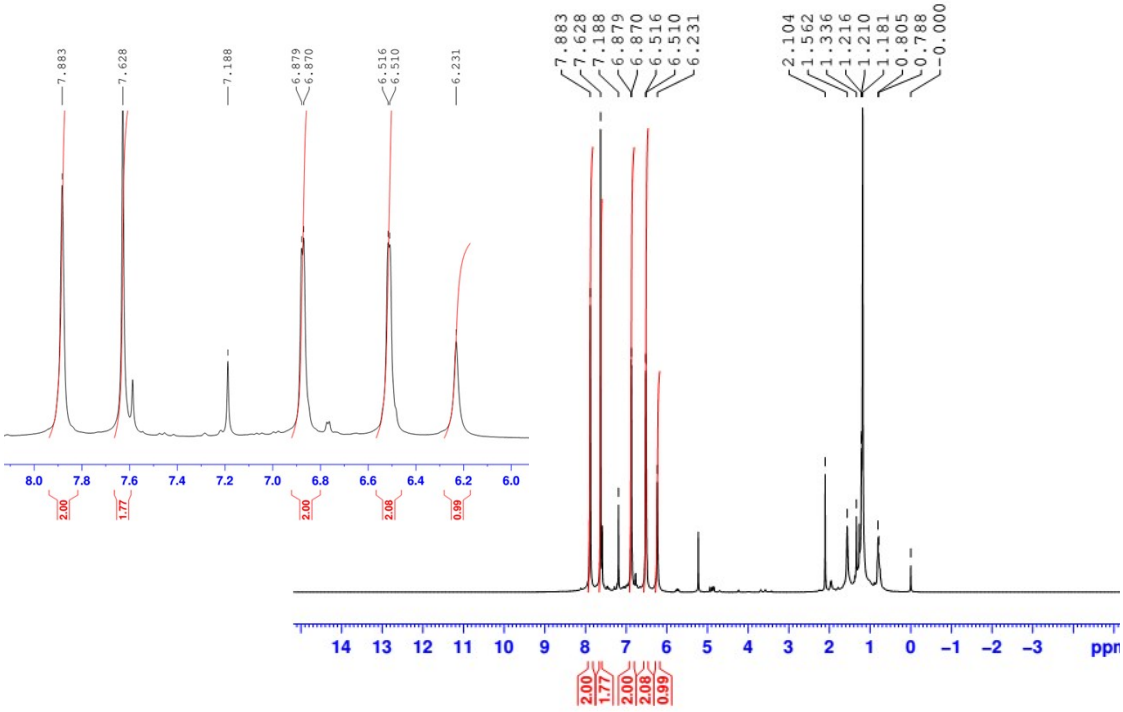

Figure S15. ^{1}H NMR spectrum of compound, **5b**.

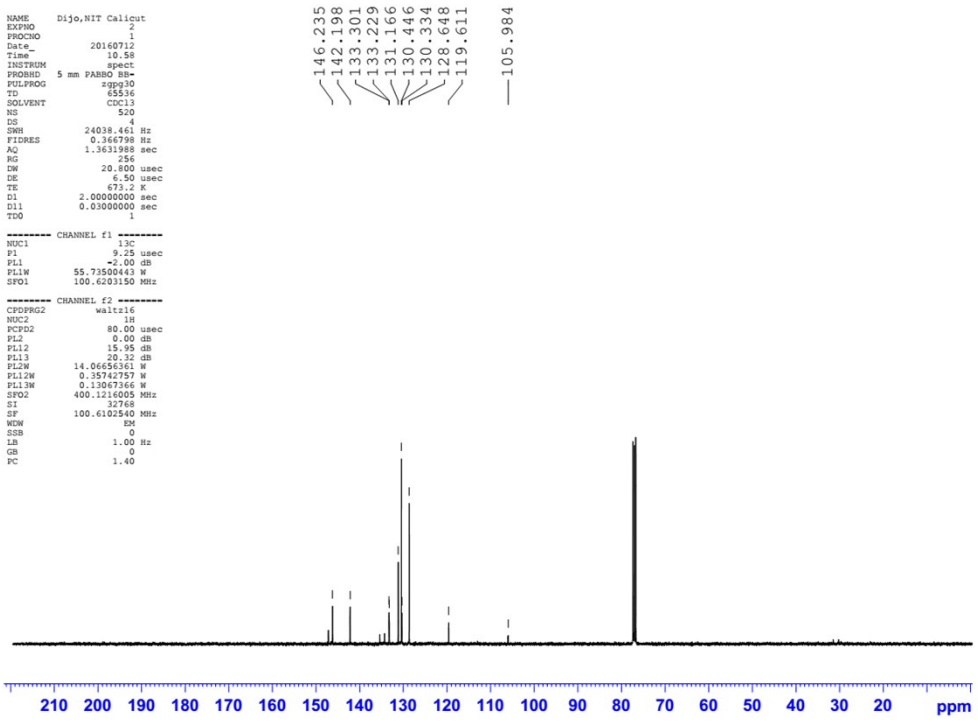

Figure S16. ^{13}C NMR spectrum of compound, **1a**.

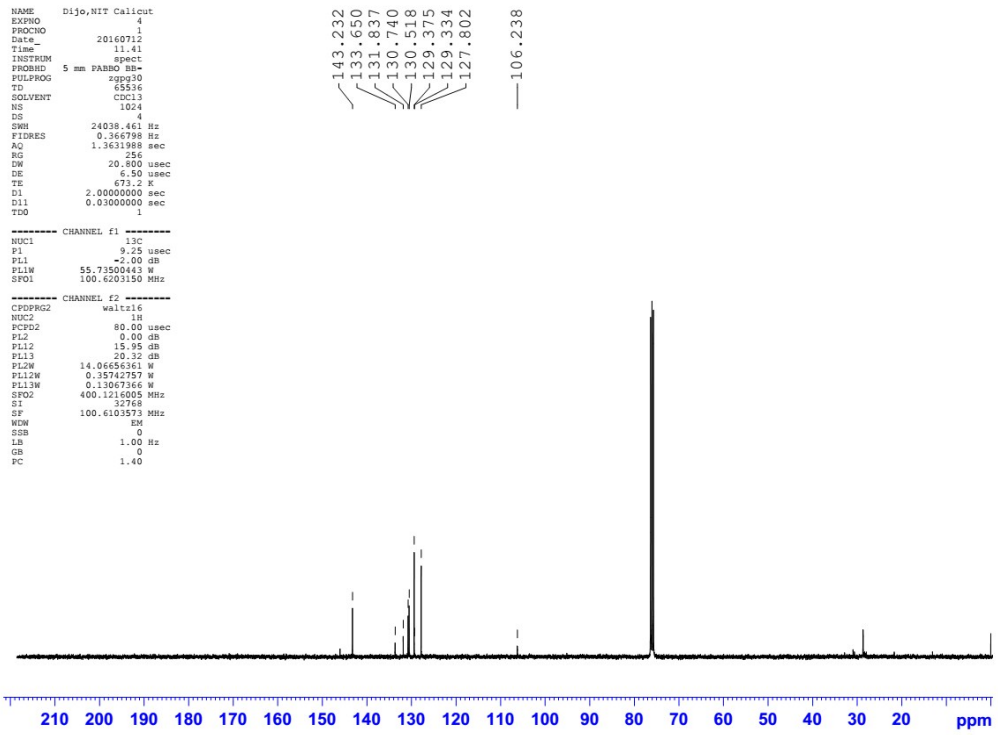

Figure S17. ^{13}C NMR spectrum of compound, **1b**.

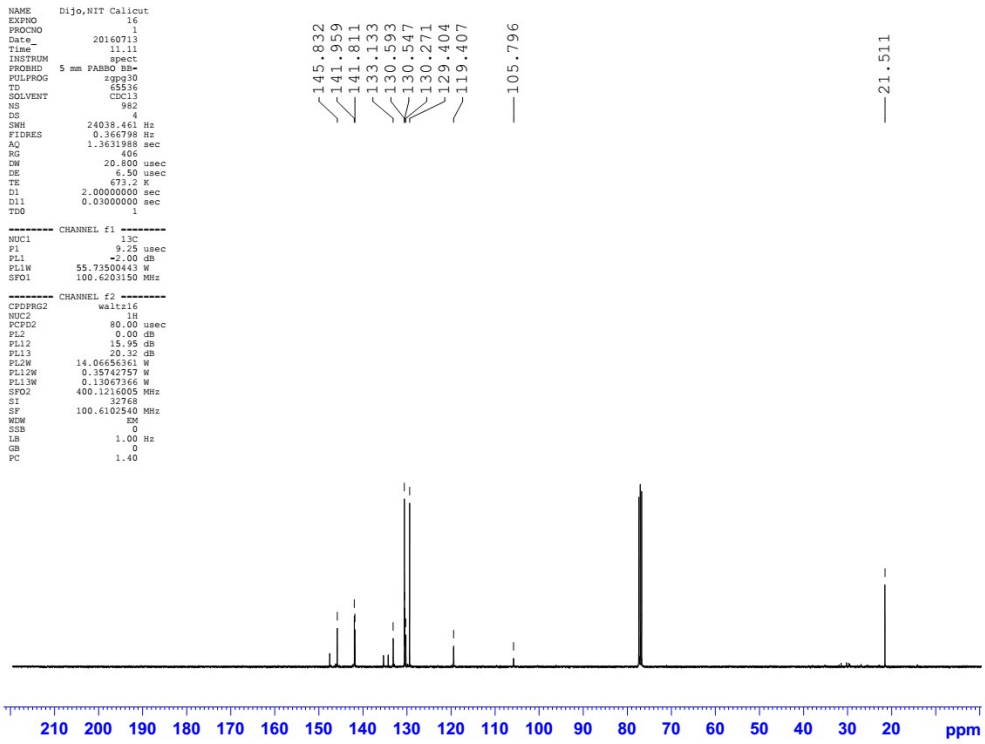

Figure S18. ^{13}C NMR spectrum of compound, **2a**.

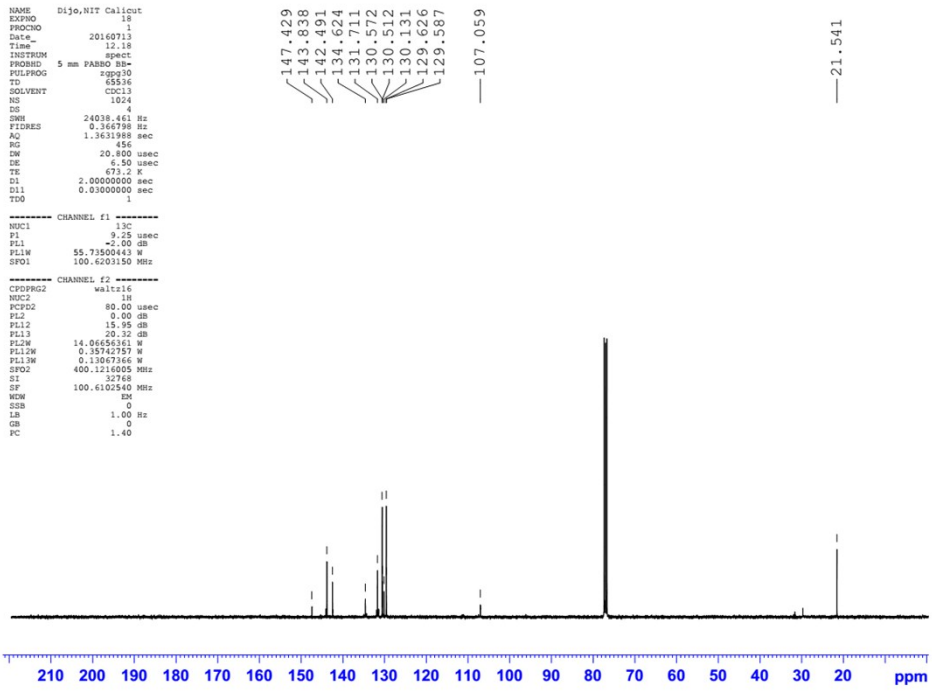

Figure S19. ^{13}C NMR spectrum of compound, **2b**.

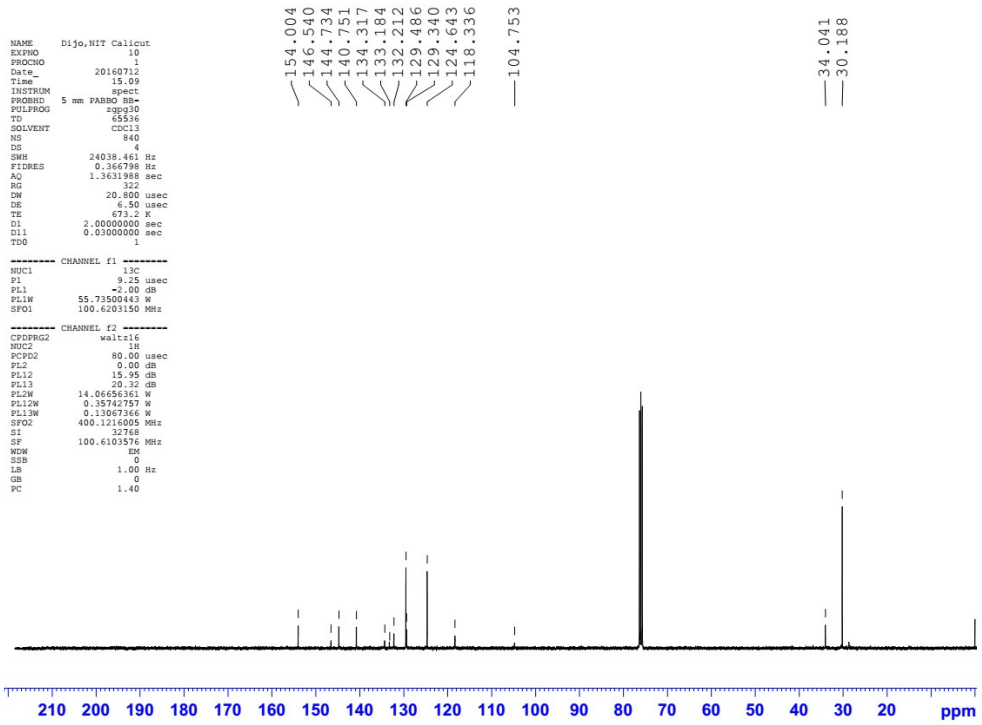

Figure S20. ^{13}C NMR spectrum of compound, **3a**.

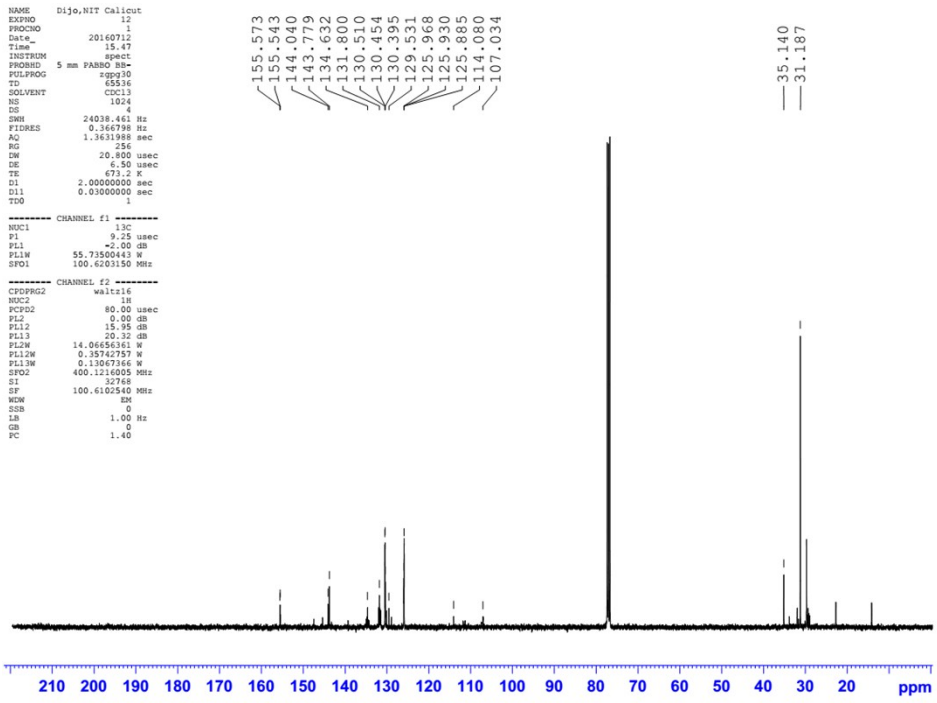

Figure S21. ^{13}C NMR spectrum of compound, **3b**.

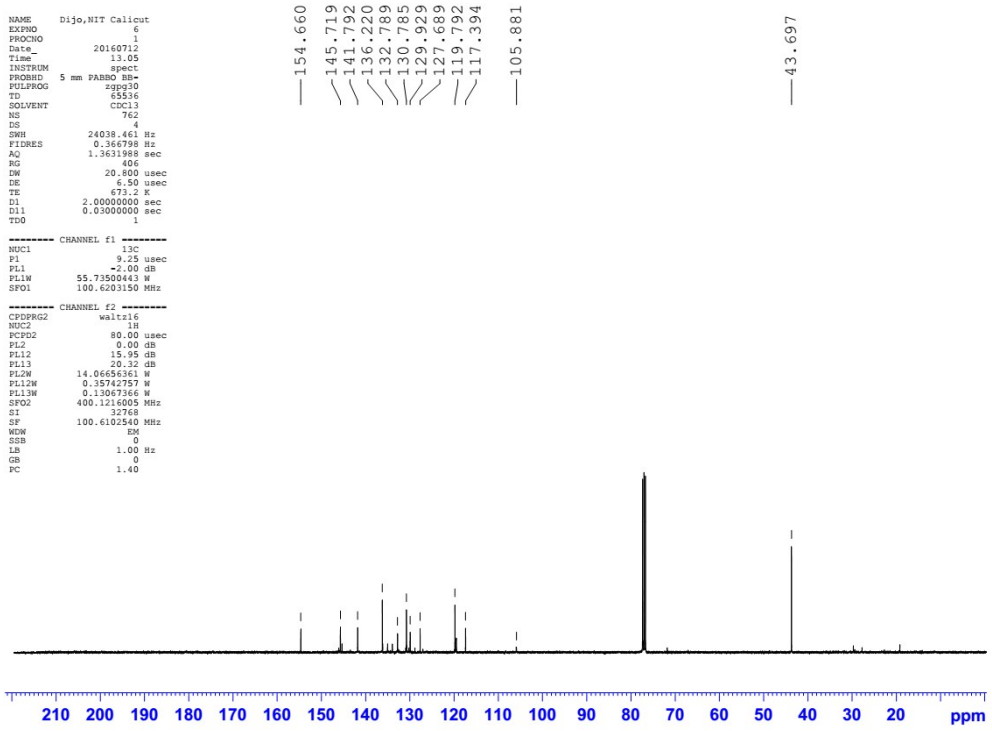

Figure S22. ^{13}C NMR spectrum of compound, **4a**.

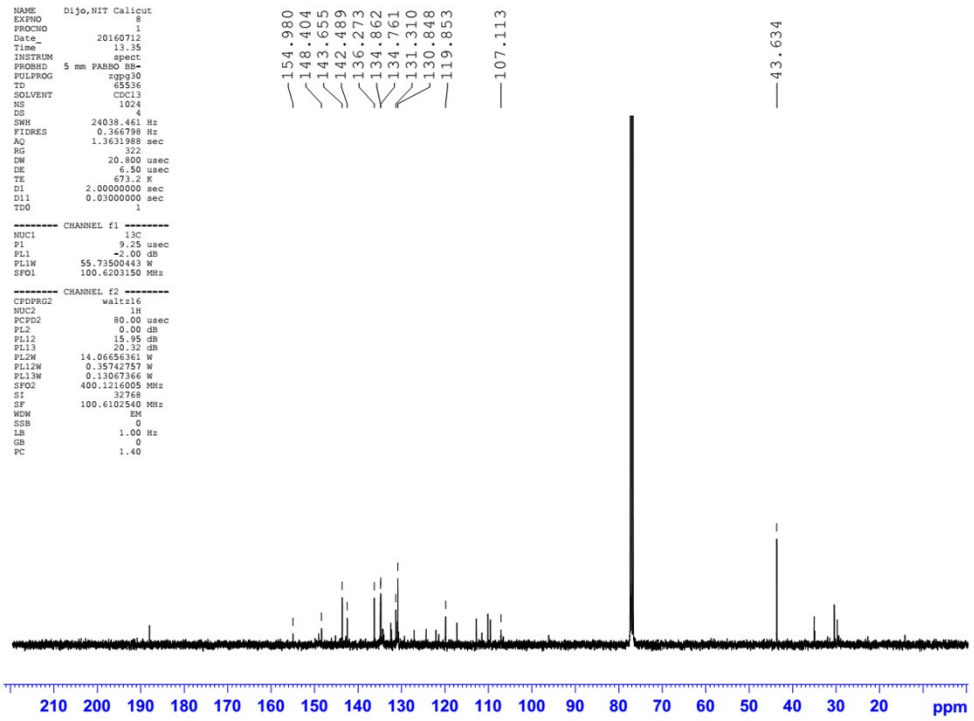

Figure S23. ^{13}C NMR spectrum of compound, **4b**.

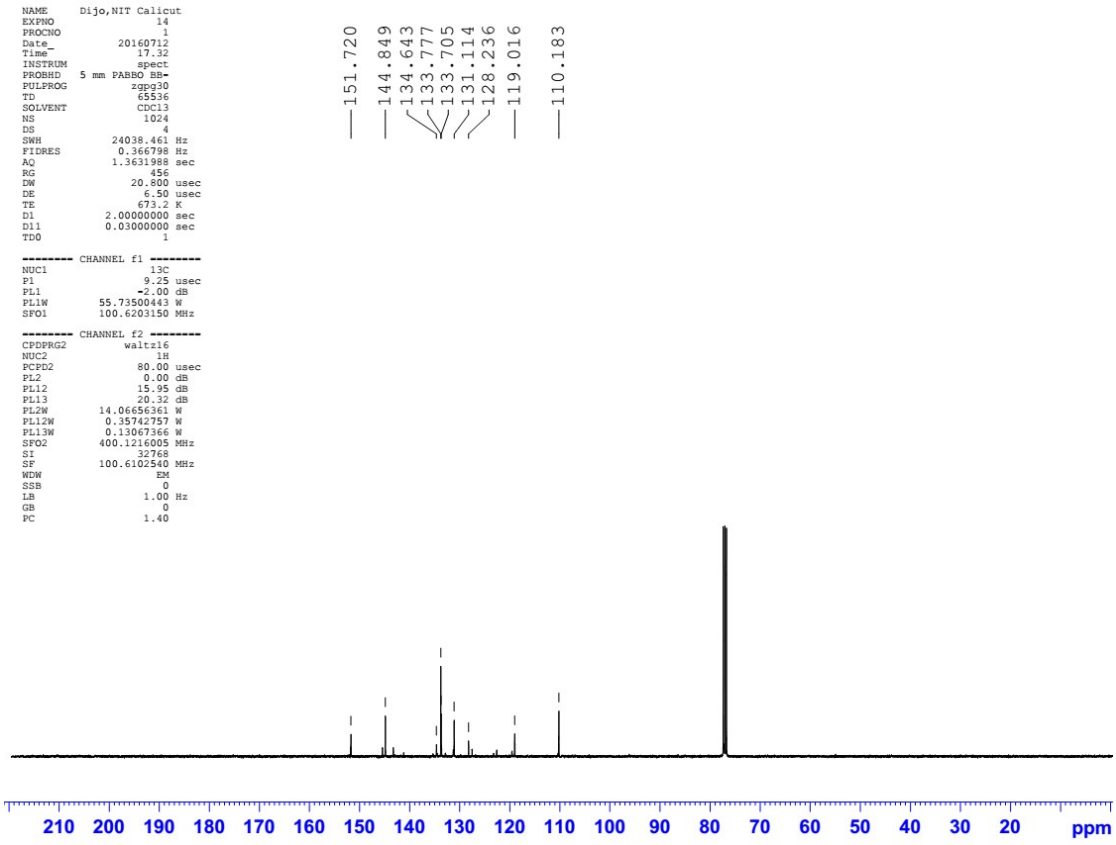

Figure S24. ^{13}C NMR spectrum of compound, **5b**.

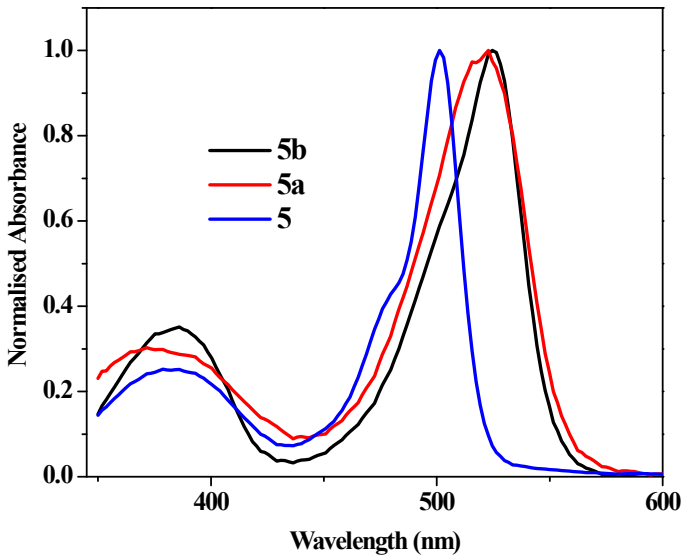

Figure S25. Absorbance spectra of compounds **5**, **5a** and **5b** in dichloromethane.

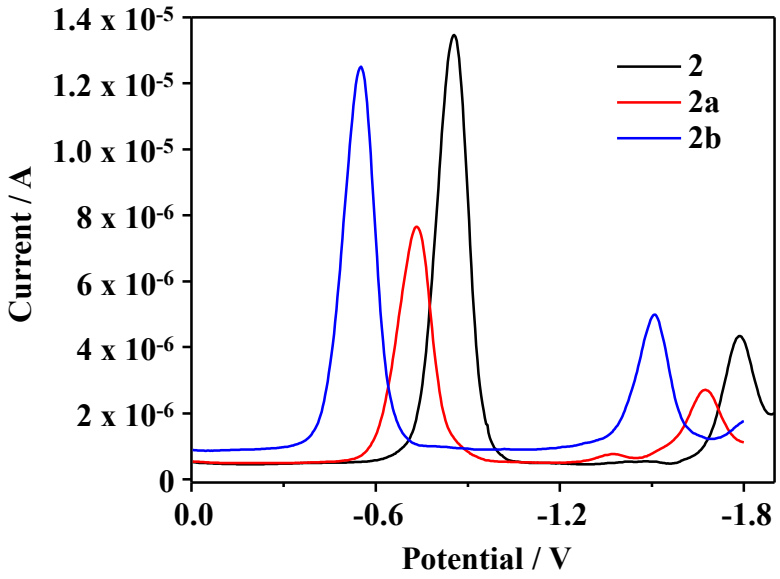

Figure S26. Differential pulse voltammograms of compounds **2**, **2a** and **2b** in dichloromethane.

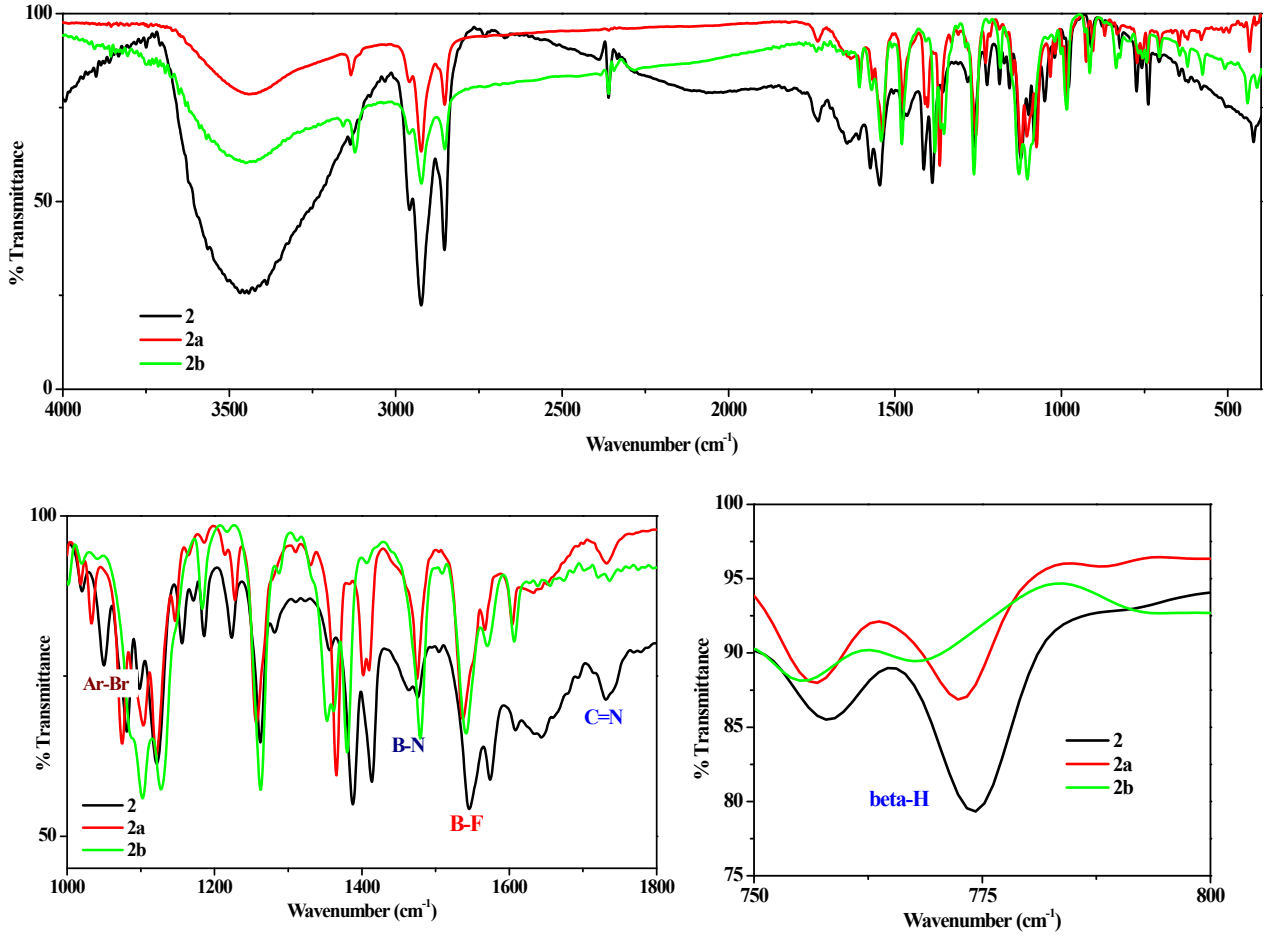

Figure S27. Comparison of IR spectra of compounds **2**, **2a** and **2b**.

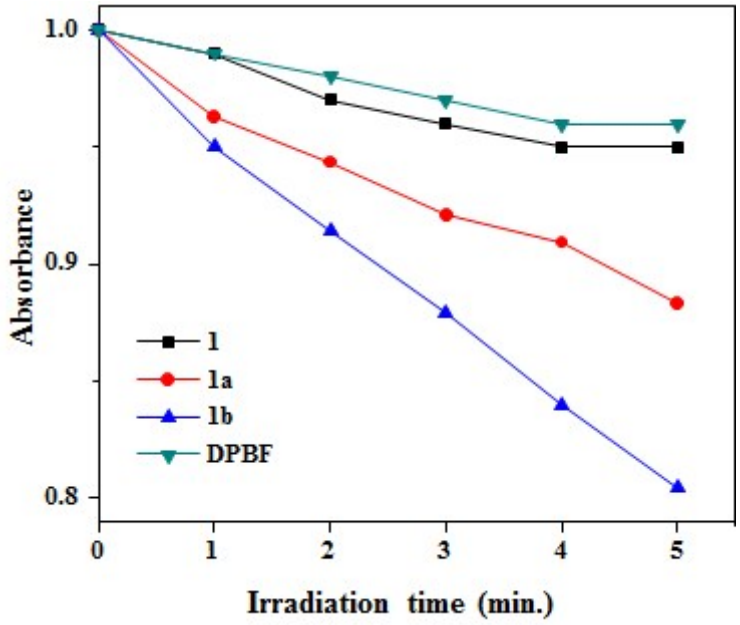

Figure S28.Plot of change in absorbance of DPBF *vs.* irradiation time in the presence of **1**, **1a** and **1b**.

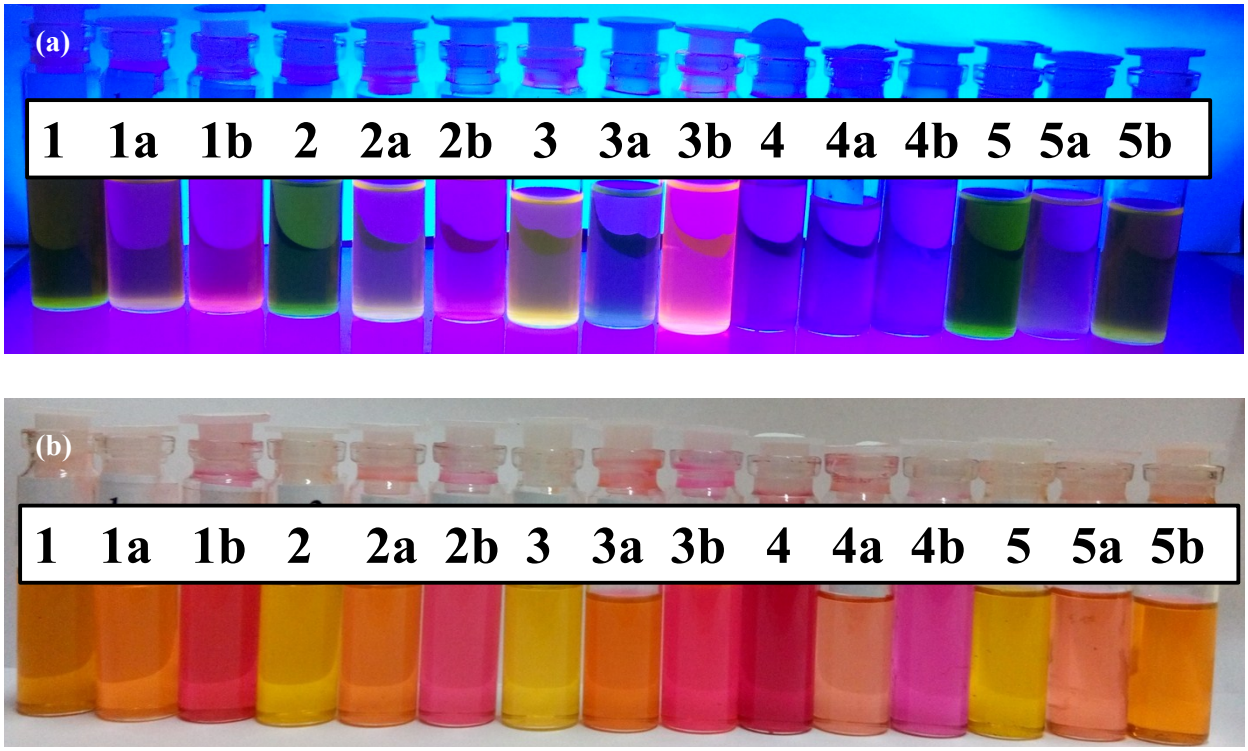

Figure S29. Photo-images of BODIPYs in CH_2Cl_2under (a) UV and (b) visible light.

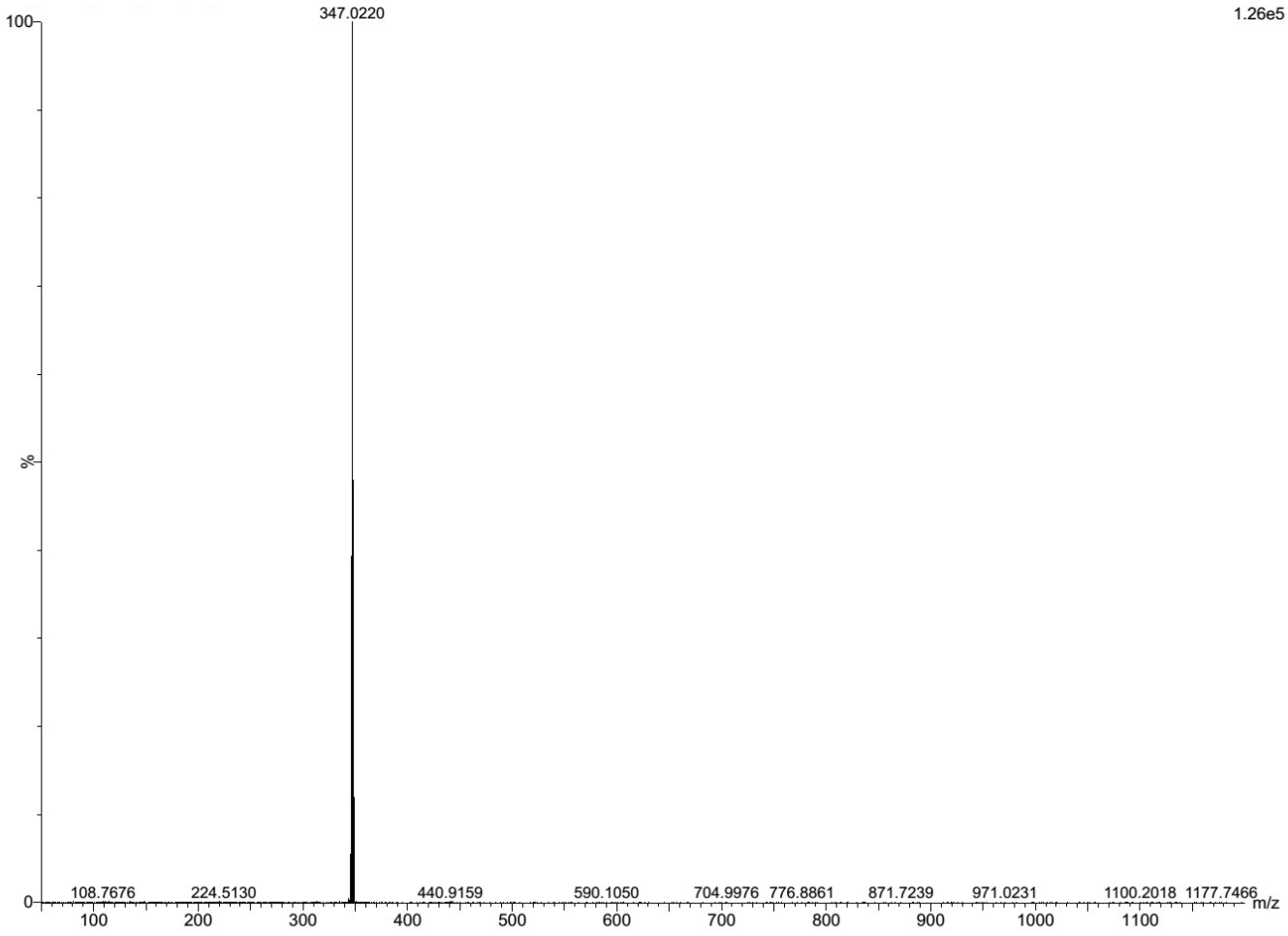

Figure S30. Mass spectrum of compound **1a**

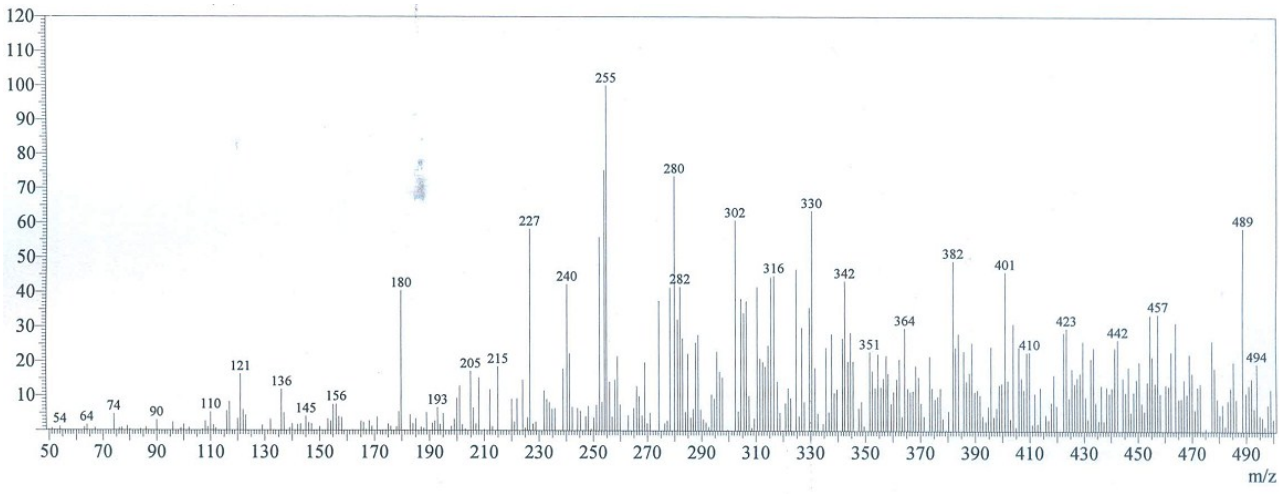

Figure S31. Mass spectrum of compound **1b**

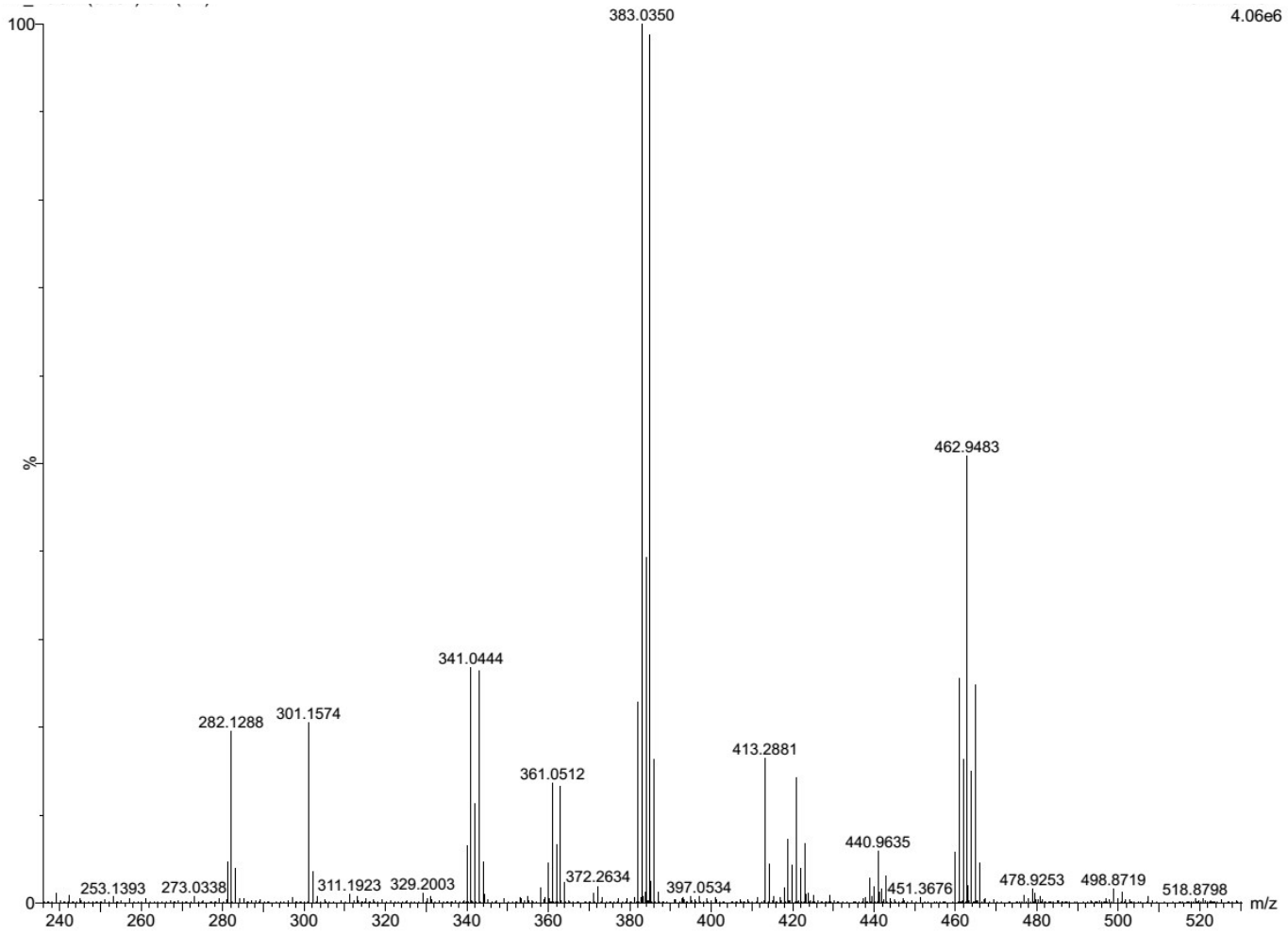

Figure S32. Mass spectrum of compound **2a**

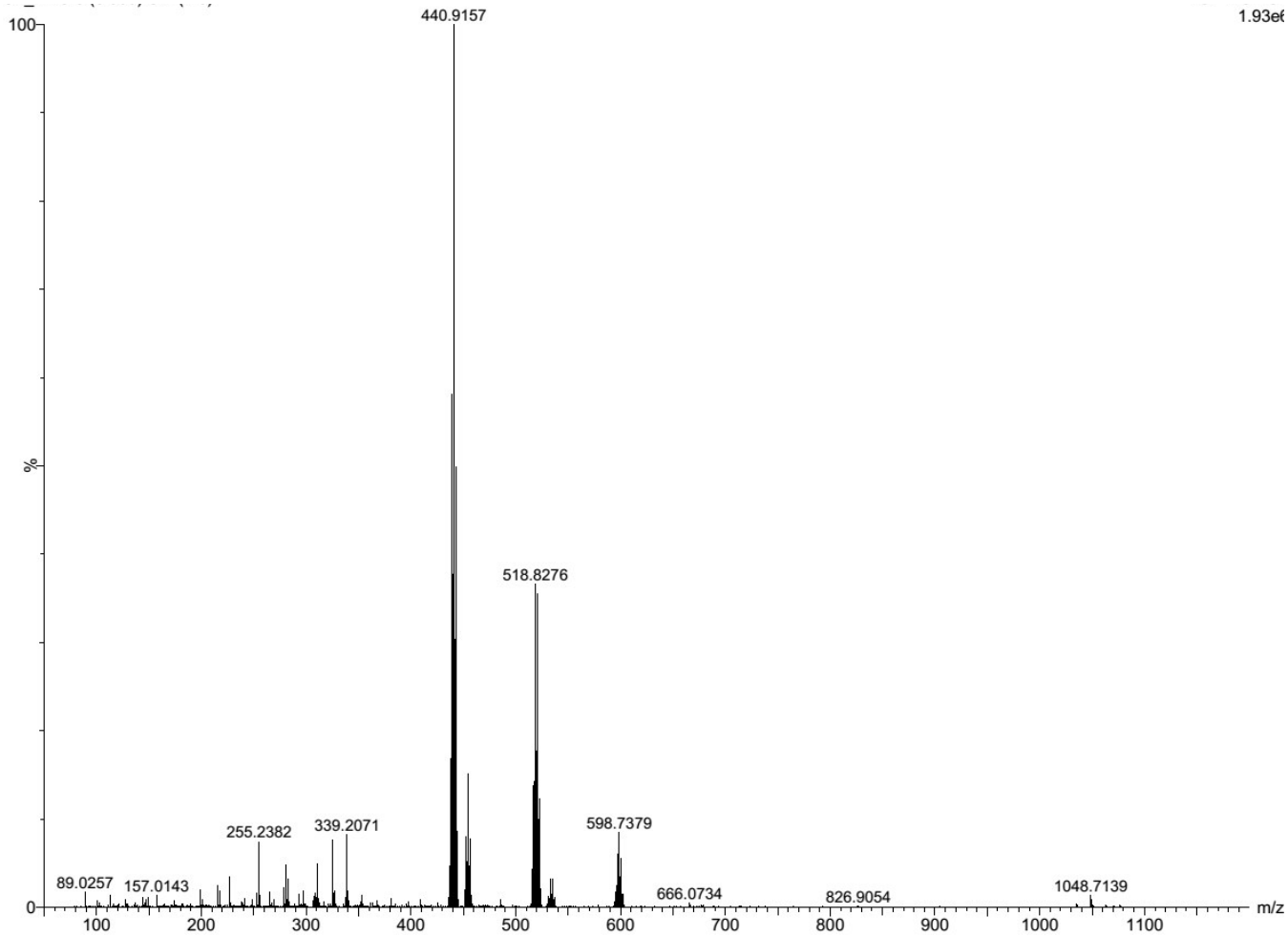

Figure S33. Mass spectrum of compound **2b**

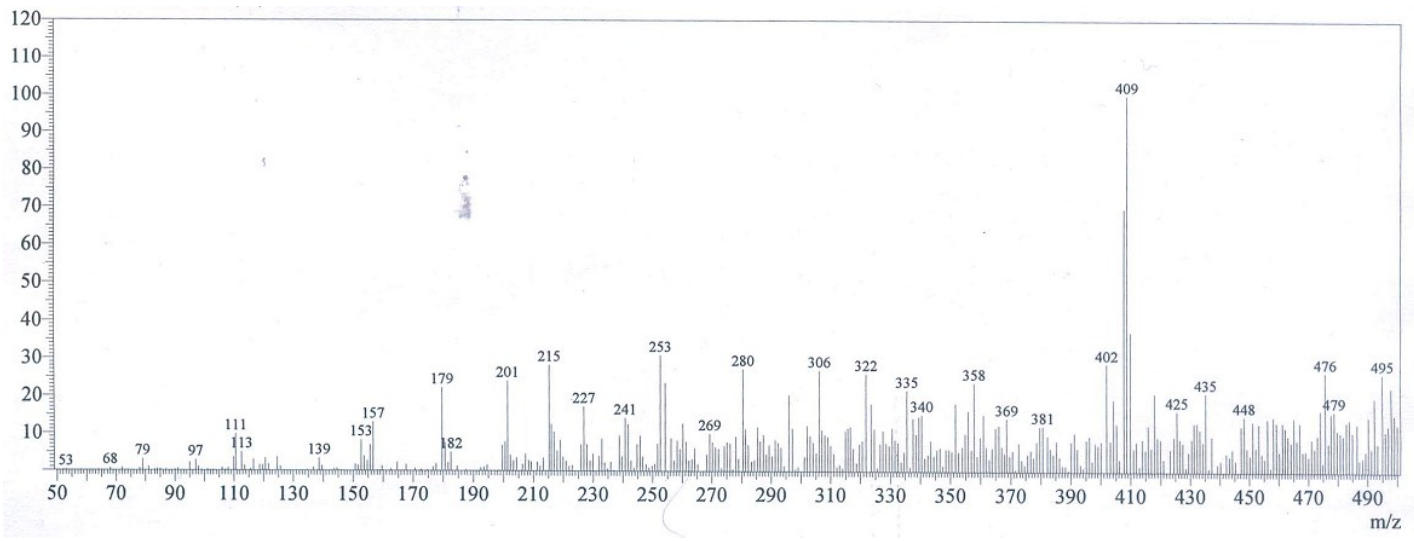

Figure S34. Mass spectrum of compound **3a**

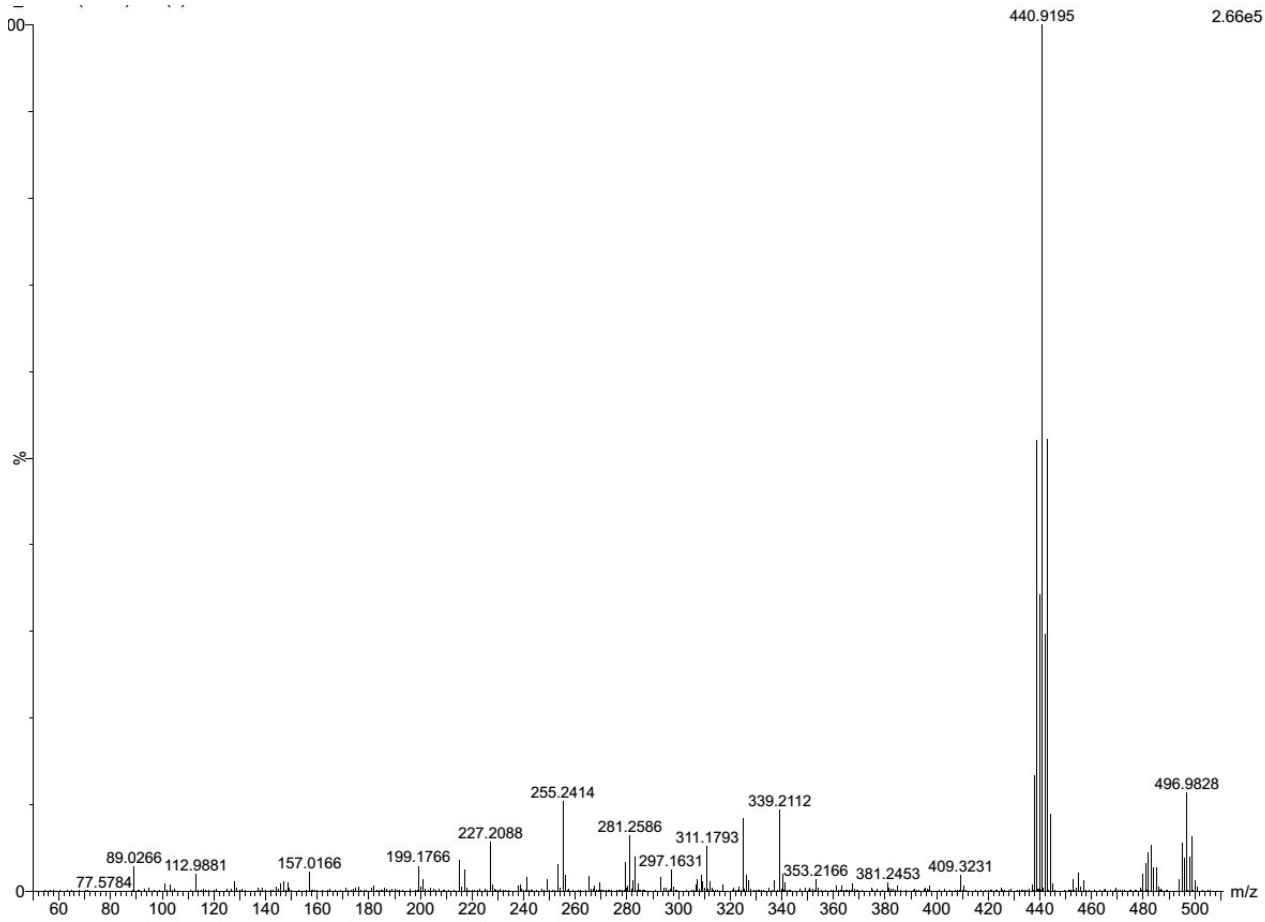

Figure S35. Mass spectrum of compound **3b**

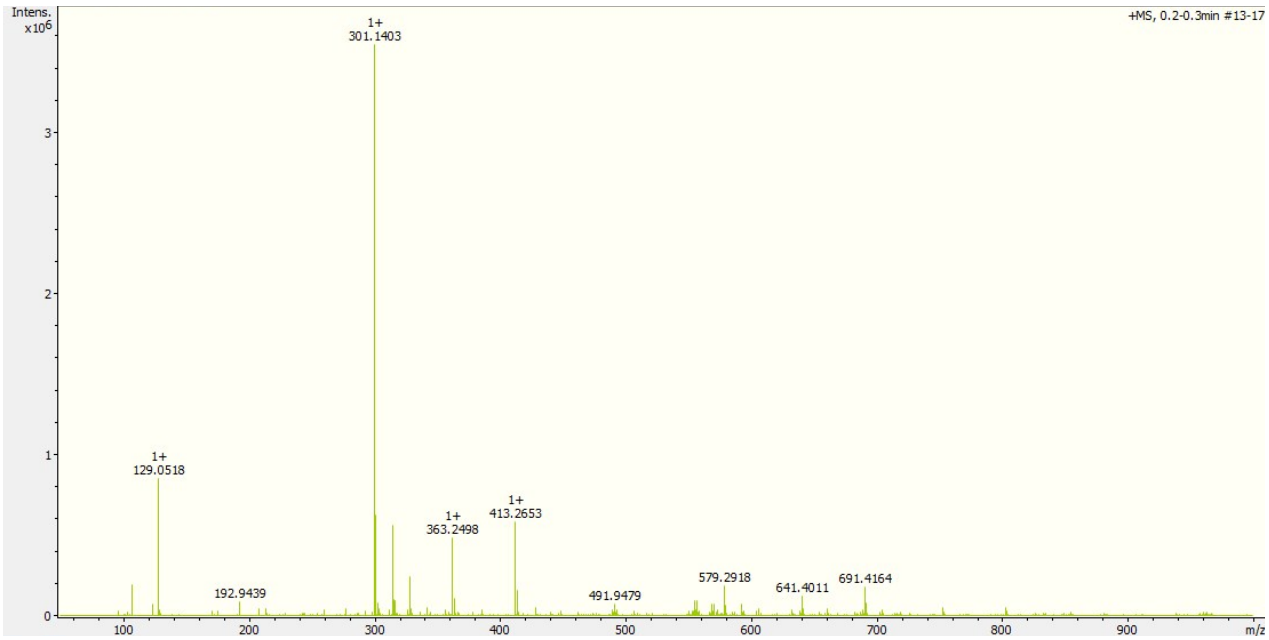

Figure S36. Mass spectrum of compound **4a**

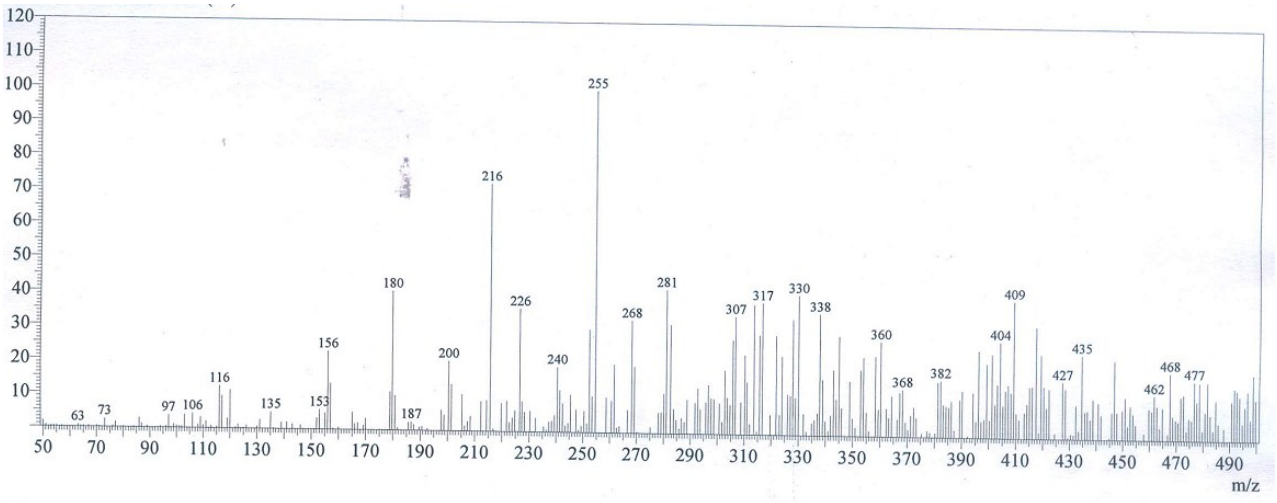

Figure S37. Mass spectrum of compound **4b**

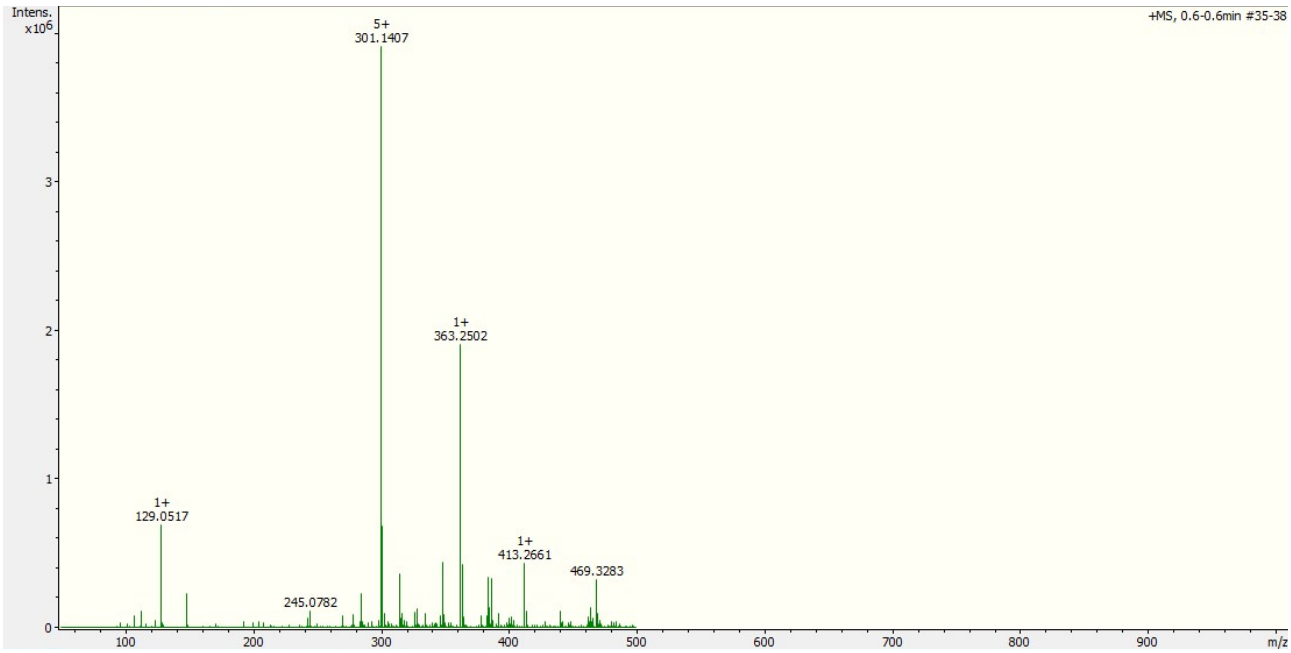

Figure S38. Mass spectrum of compound **5a**

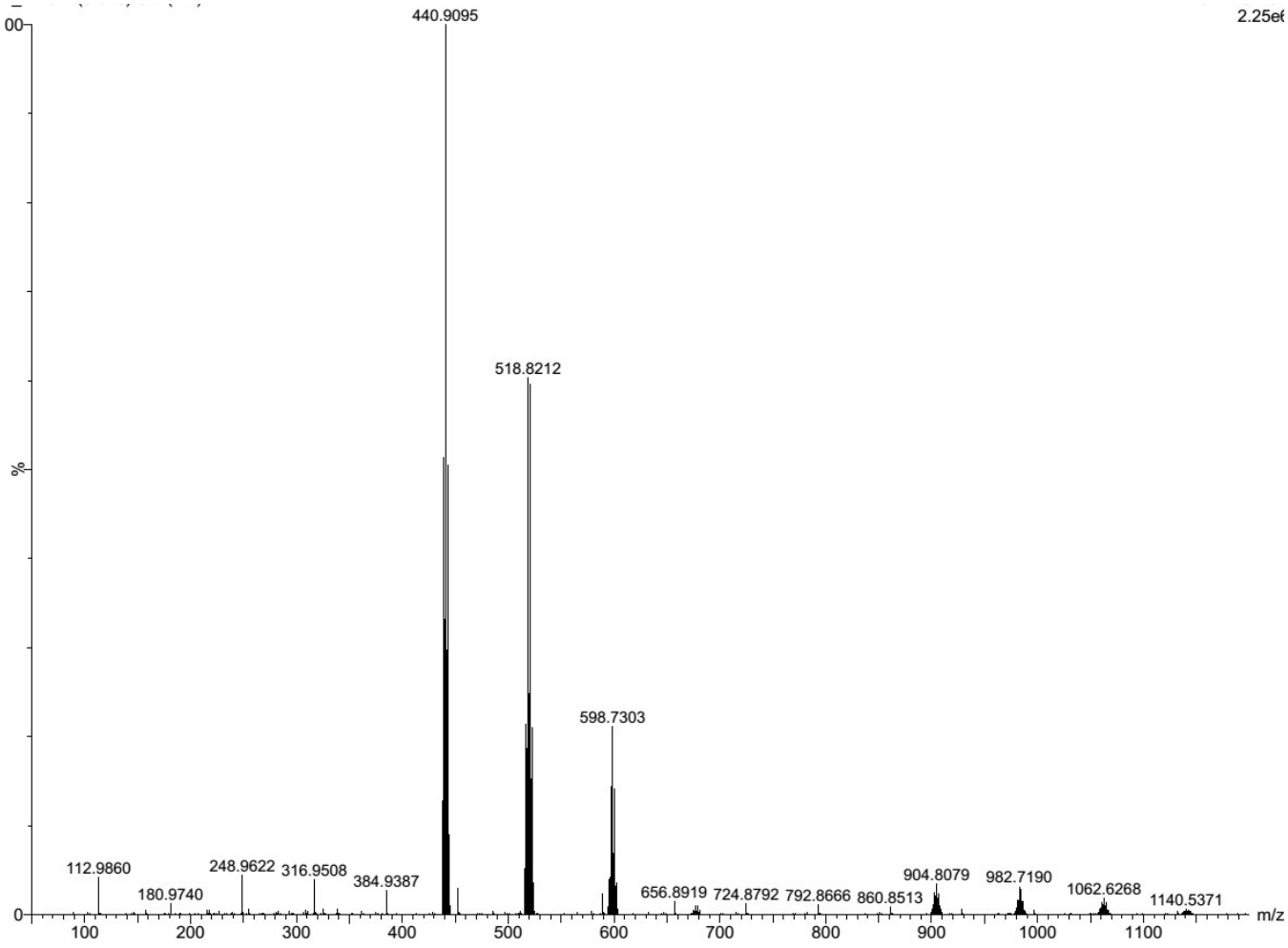

Figure S39. Mass spectrum of compound **5b**

Table S1. Solvatochromic data for compounds, **1-5**.

Compound	Solvent	λ_{max}(nm)	λ_{em}(nm)	Stokes shift, Δ_{max} (cm^{-1})	Compound	Solvent	λ_{max}(nm)	λ_{em}(nm)	Stokes shift, Δ_{max} (cm^{-1})
1[i]	MeOH	497	514	665	**3b**	MeOH	539	560	696
	MeCN	496	513	668		MeCN	538	560	730
	THF	499	516	660		THF	542	562	657
	Toluene	501	522	810		Toluene	544	564	652
1a[i]	MeOH	512	537	909	**4**	MeOH	488	-	-
	MeCN	511	537	947		MeCN	483	-	-
	THF	515	540	899		THF	492	543	1868
	Toluene	521	543	778		Toluene	498	626	4068
1b[i]	MeOH	533	556	776	**4a**	MeOH	514	546	1140
	MeCN	531	557	879		MeCN	516	549	1165
	THF	535	558	770		THF	516	549	1165
	Toluene	540	565	819		Toluene	521	613	2881
2	MeOH	496	511	573	**4b**	MeOH	531	559	943
	MeCN	495	510	594		MeCN	528	559	1050
	THF	498	512	549		THF	532	547	515
	Toluene	501	518	655		Toluene	536	608.5	2236
2a	MeOH	511	535	878	**5**	MeOH	493	508	599
	MeCN	509	536	989		MeCN	493	508	599
	THF	513	537	871		THF	495	510	594
	Toluene	518	540	787		Toluene	501	518	655
2b	MeOH	532	555	779	**5a**	MeOH	507	536	1067
	MeCN	530	555	849		MeCN	510	535	916
	THF	533	557	808		THF	512	539	978
	Toluene	538	560	730		Toluene	519	545	919
3	MeOH	495	512	671	**5b**	MeOH	490	521	1214
	MeCN	495	512	671		MeCN	504	516	461
	THF	499	515	623		THF	507	526	712
	Toluene	501	520	729		Toluene	512	532	734
3a	MeOH	511	535	878					
	MeCN	510	536	951					
	THF	514	538	868					
	Toluene	518	541	820					

[i]Absorption of **1**, **1a** and **1b** in toluene (X.-F. Zhangand X. Yang, *J. Phys. Chem. B.,* 2013, 117, 5533-5539) and photophysical properties of **1**, **1a** and **1b** in acetonitrile, methanol and toluene at room temperature at λ_{ex}= 494, 493 and 501 nm respectively (M. Baruah*et al*., *J. Org. Chem.,*2005, 70, 4152-4157).

Table S2. Distances (in Å) for different types of interactions in BODIPYs, **1**, **2**, **2a, 3**, **5** and **5b**.

Interaction[i]	1[ii]	2[ii]	2a[ii]	3[ii]	5[ii]	5b[ii]
$C_{(Pyr)}\cdots C_{(Ph)}$	3.298 (**2**)	-	-	-	3.370 (**2**)	-
$C_{(Pyr)}\cdots C_{(Pyr)}$	3.348-3.398 (**3**)	-	3.386	-	-	-
N-B$\cdots C_{(Ph)}$	3.748 (**2**)	-	-	-	-	-
N-B$\cdots H_{(Ph)}$	3.022	-	-	-	3.072 (**2**)	-
N-B$\cdots H_{(Sol)}$	2.968 (**2**)	-	-	-	2.754 (**2**)	3.098 (**2**)
N-B$\cdots H_{(Pyr)}$	3.100	-	3.042 (**2**)	-	-	-
B-F$\cdots H_{(Ph)}$	2.623-2.654 (**3**)	2.554 (**2**)	2.631 (**2**)	2.533-2.578 (**4**)	2.638 (**2**)	-
B-F$\cdots H_{(Me)}$	-	2.602 (**2**)	-	-	-	-
B-F$\cdots H_{(Sol)}$	2.407 (**2**)	-	-	-	1.942 (**2**)	-
B-F$\cdots H_{(Hydroxy)}$	-	-	-	-	-	1.988 (**2**)
B-F$\cdots H_{(Pyr)}$	2.348-2.562 (**5**)	-	2.359-2.640 (**4**)	-	-	2.484 (**2**)
B-F$\cdots O_{(Sol)}$	-	-	-	-	2.838 (**2**)	-
B-F$\cdots O_{(Hydroxy)}$	-	-	-	-	-	2.731 (**2**)
B-F$\cdots C_{(Ph)}$	2.982 (**2**)	-	-	-	-	3.147 (**2**)
B-F$\cdots C_{(Pyr)}$	3.120 (**2**)	-	-	-	-	-
N-B$\cdots O_{(Sol)}$	-	-	-	-	3.501 (**2**)	-
$_{(Hydroxy)}O\cdots O_{(Sol)}$	-	-	-	-	2.627- 2.791 (**4**)	-
$_{(Hydroxy)}H\cdots O_{(Sol)}$	-	-	-	-	1.818 (**2**)	-
$_{(Sol)}H\cdots O_{(Hydroxy)}$	-	-	-	-	1.878 (**2**)	-
$_{(Hydroxy)}H\cdots H_{(Sol)}$	-	-	-	-	2.272-2.395 (**4**)	-
$_{(Pyr)}H\cdots H_{(Pyr)}$	-	2.338	-	-	-	-
$_{(Sol)}H\cdots C_{(Ph)}$	-	-	-	-	2.597 (**2**)	-
$_{(Ph)}H\cdots C_{(Pyr)}$	-	-	-	-	-	2.757 (**2**)
$_{(Ph)}H\cdots C_{(Ph)}$	2.818 (**2**)	-	-	-	-	-
$_{(Pyr)}H\cdots C_{(Ph)}$	2.754-2.886 (**4**)	2.865 (**2**)	-	-	-	-
$_{(Pyr)}Br\cdots C_{(Ph)}$	-	-	3.449 (**2**)	-	-	-
$_{(Ph)}Br\cdots C_{(Pyr)}$	-	-	-	-	-	3.361 (**2**)
$_{(Ph)}Br\cdots H_{(Pyr)}$	-	-	-	-	-	2.946 (**2**)
$_{(Pyr)}N\cdots H_{(Ph)}$	2.737	-	-	-	-	-

[i]Different types. [ii]Value in parenthesis gives the number of interactions present in the molecule.

Table S3. Comparison of IC_{50} values of different BODIPYs against *BS* and *EC*.

Compound	IC_{50} in *BS (μM)*	IC_{50} in *EC (μM)*	Compound	IC_{50} in *BS (μM)*	IC_{50} in *EC (μM)*
1	27	-	**3b**	12	-
1a	21	34	**4**	18	38
1b	20	34	**4a**	10	41
2	36	-	**4b**	6	34
2a	10	22	**5**	18	17
2b	13	38	**5a**	10	25
3	-	-	**5b**	5	26
3a	8	-	**-**	-	-