Electronic Supplementary Information for

BOSCHIBAs as a fluorescent dye of silk fibroin with mechano- and thermoresistive properties: ultrasound synthesis, photophysical characterization, X-ray analysis, and molecular docking

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Table S1. Synthesis parameters with ultrasonic radiation for the ligands and BOSCHIBAs, at room temperature.

LIGANDS	TIME	YIELD	BOSCHIBAS	TIME	YIELD
1	2 hours	97%	**5**	4 hours	74%
2		93%	**6**		85%
3		75%	**7**		65%
4		91%	**8**		89%

Table S2. Physical properties of Ligands and BOSCHIBAs

LIGANDS	COLOR	P.F.	BOSCHIBAS	COLOR	P.F.
1	Yellow	216°C	**5**	Yellow	180°C
2	Red	211°C	**6**	Pink	191°C
3	White	151°C	**7**	Yellow	159°C
4	Yellow	241°C	**8**	Yellow	251°C

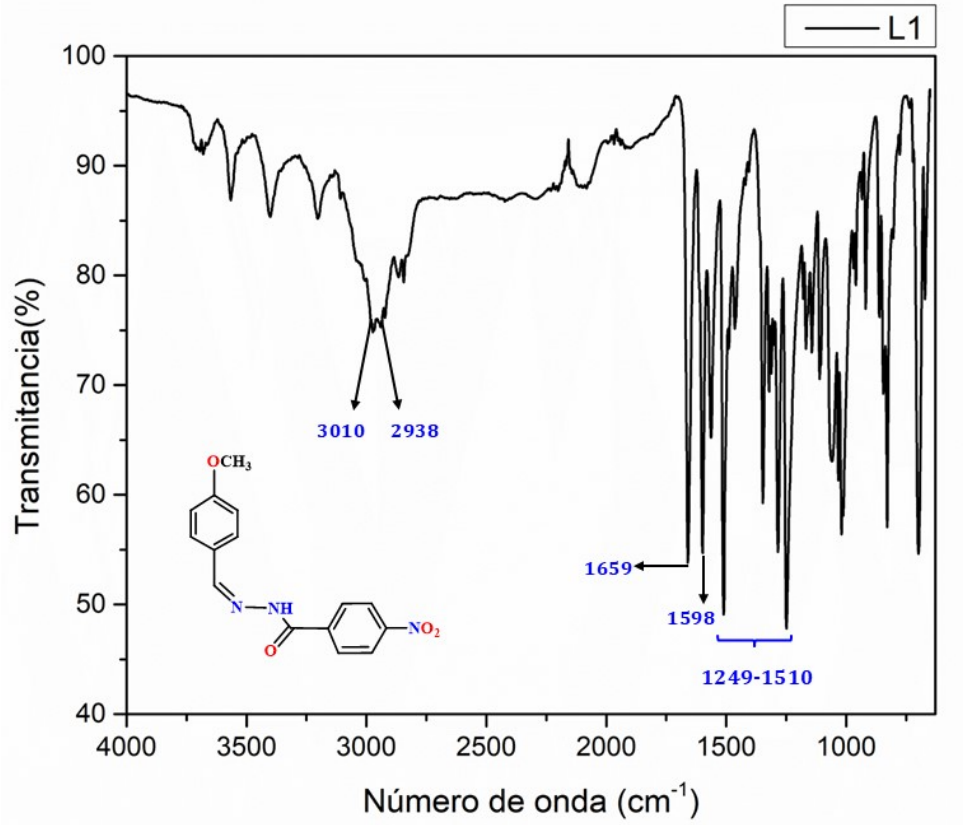

Figure S1. IR spectrum of ligand **1**.

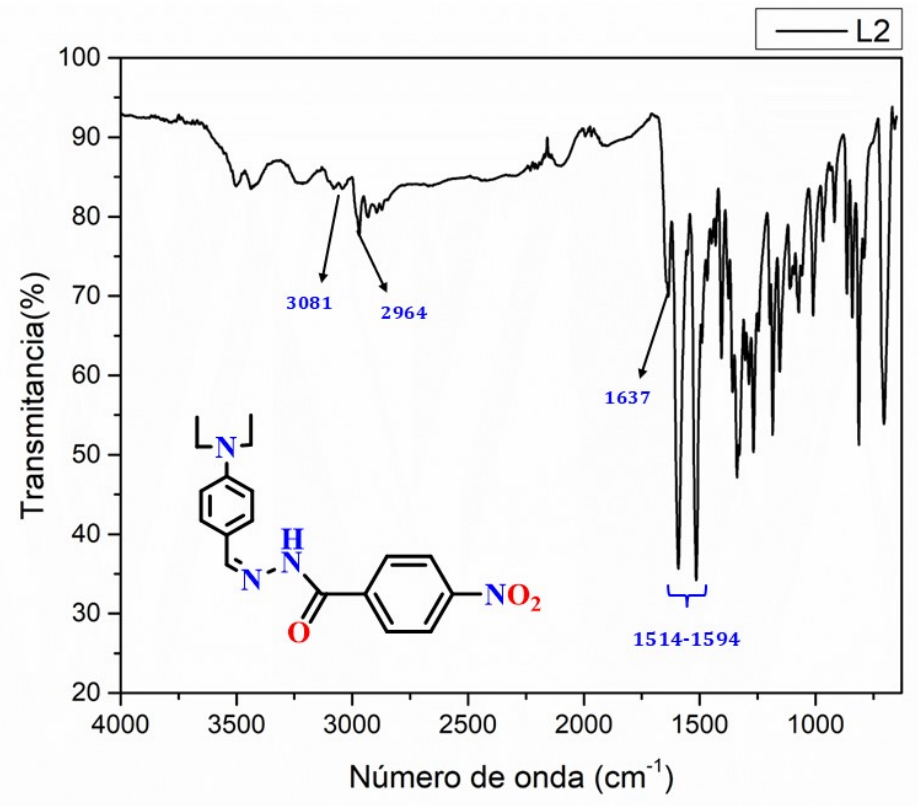

Figure S2. IR spectrum of ligand **2**

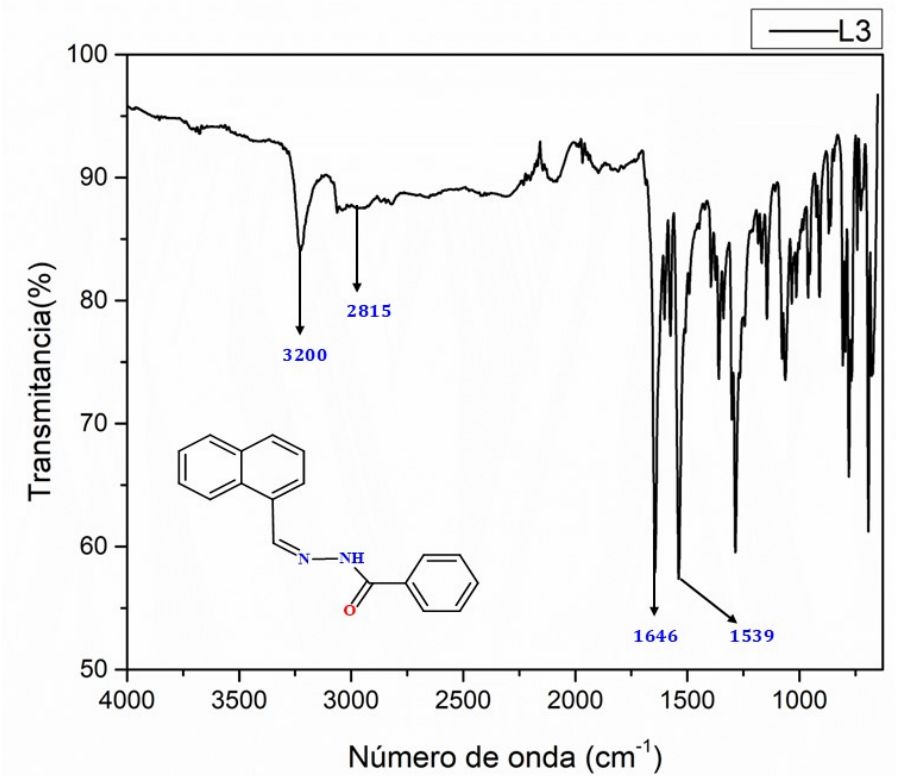

Figure S3. IR spectrum of ligand **3**

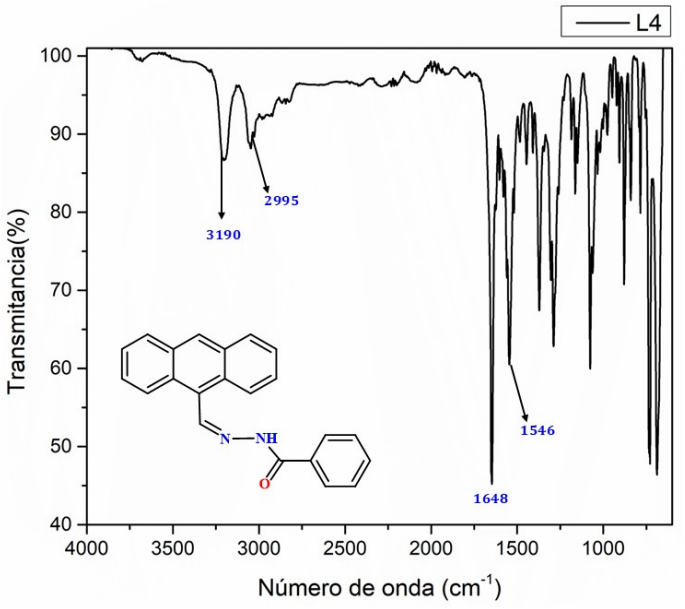

Figure S4. IR spectrum of ligand **4**

Table S3: IR data in cm^{-1} for ligands **1-4**

Ligand	υ(C=N)	υ(C=O)	υ(ES-NO_2)	υ(N-N)	υ(C-Har)
1	1659	1598	1249-1510	2938	3010
2	1637	1601	1514-1594	2964	3081
3	1646	1539		2815	3200
4	1648	1546		2995	3190

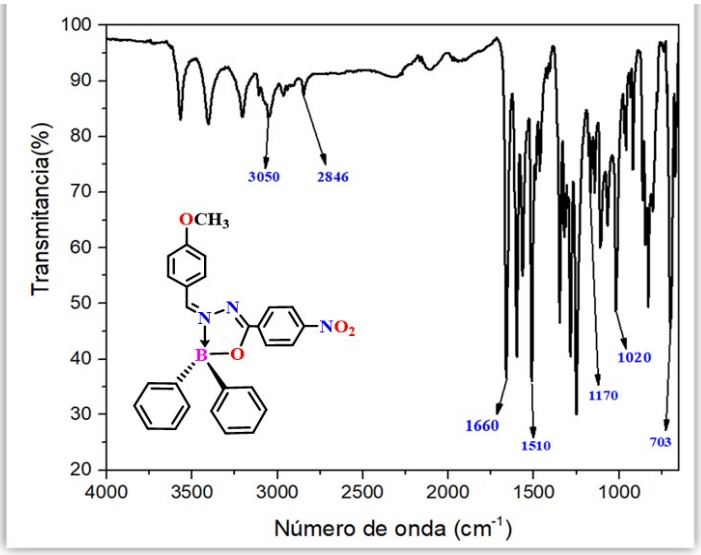

Figure S5. IR spectrum of compound **5**

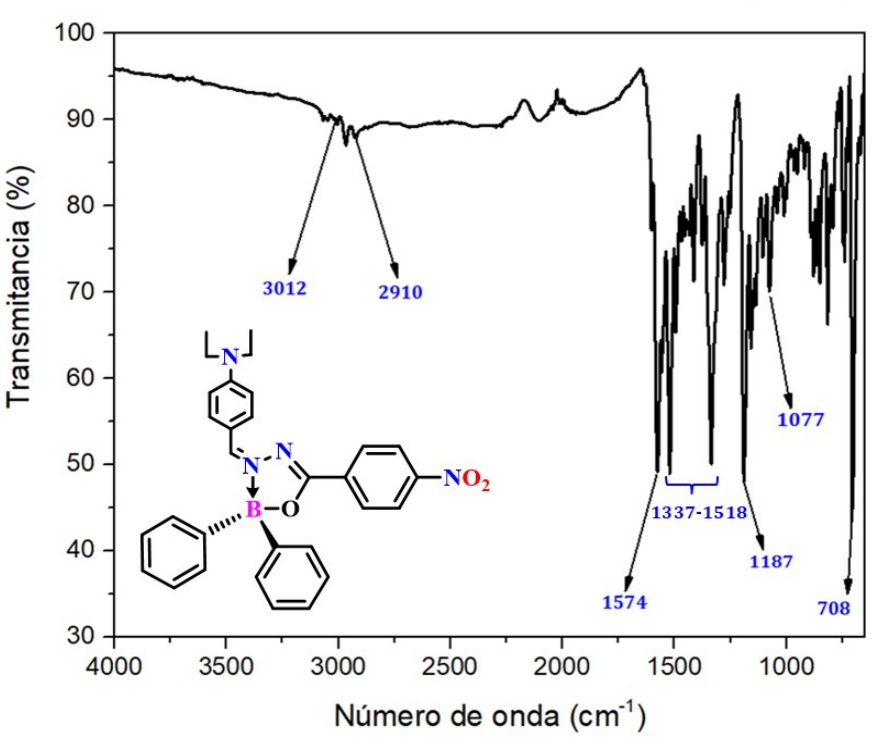

Figure S6. IR spectrum of compound **6.**

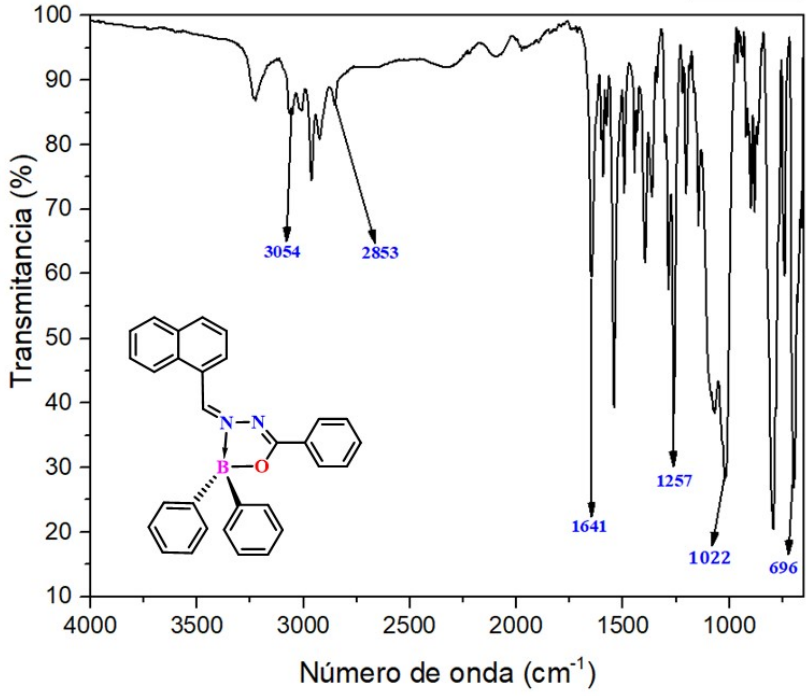

Figure S7. IR spectrum of compound **7**

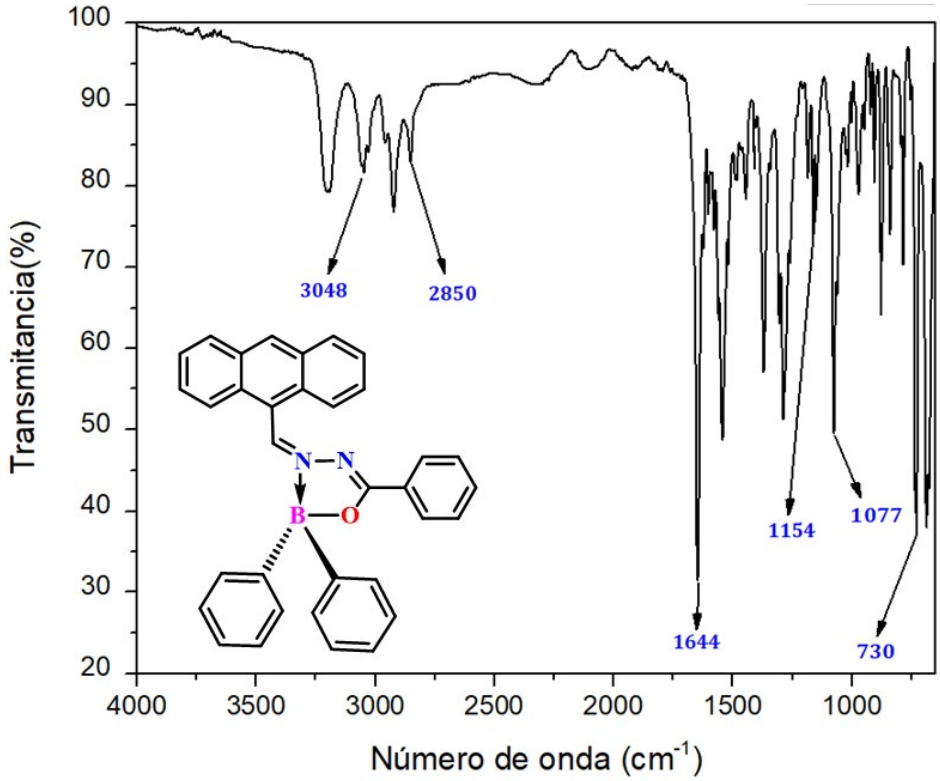

Figure S8. IR spectrum of compound **8**

Table S4: IR data in cm^{-1} of compounds **5-8**

BOSCHIBAS	υ(C=N)	υ(C-O)	υ(ES-NO_2)	υ(N-N)	υ(C-H_{AR})	υ(C-H_{AREP})	υ(C-H_{ARFP})
5	1660	1020	1343-1510	2846	3050	1170	703
6	1574	1077	1337-1518	2910	3012	1187	708
7	1641	1022	-	2853	3054	1257	696
8	1644	1077	-	2850	3048	1145	730

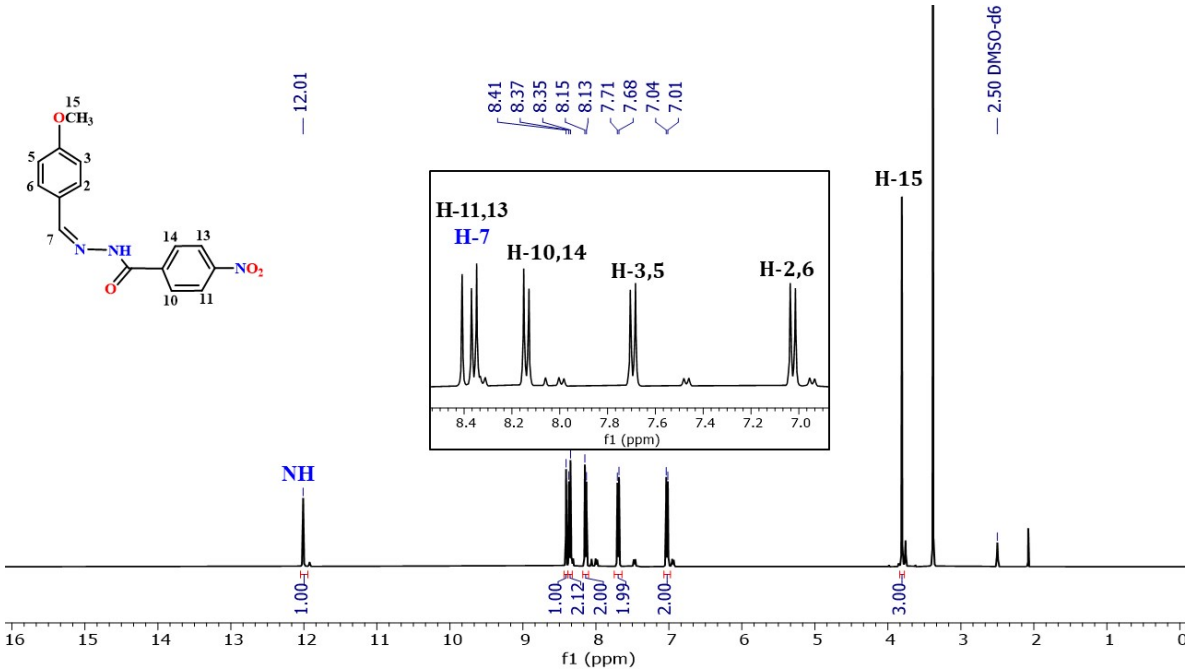

Figure S9. ^{1}H NMR Spectrum in DMSO-d_6 of ligand **1**.

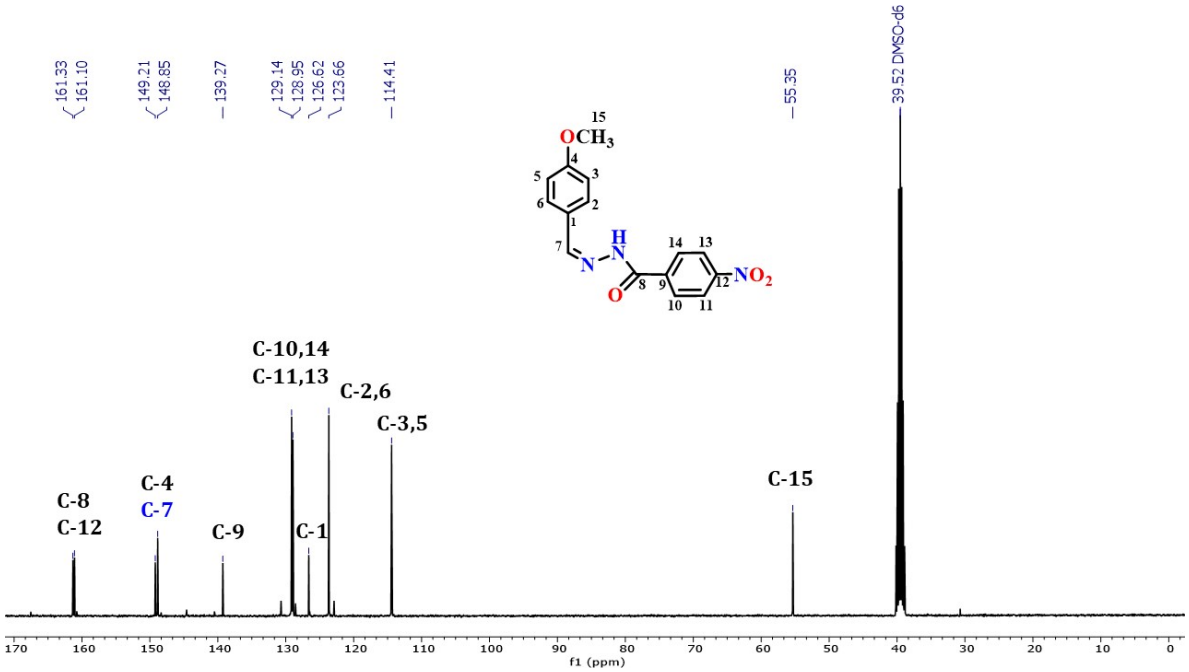

Figure S10. ^{13}C {1H} NMR Spectrum in DMSO-d_6 of ligand **1**.

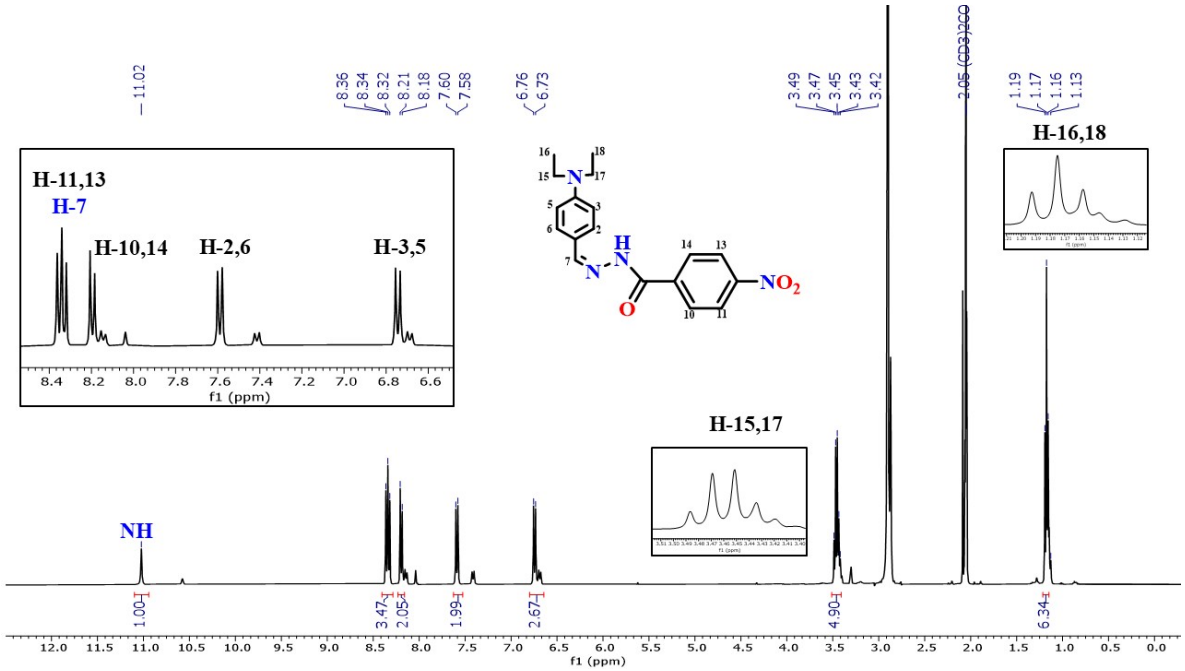

Figure S11. ^{1}H NMR Spectrum in acetone-d_6 of ligand **2**.

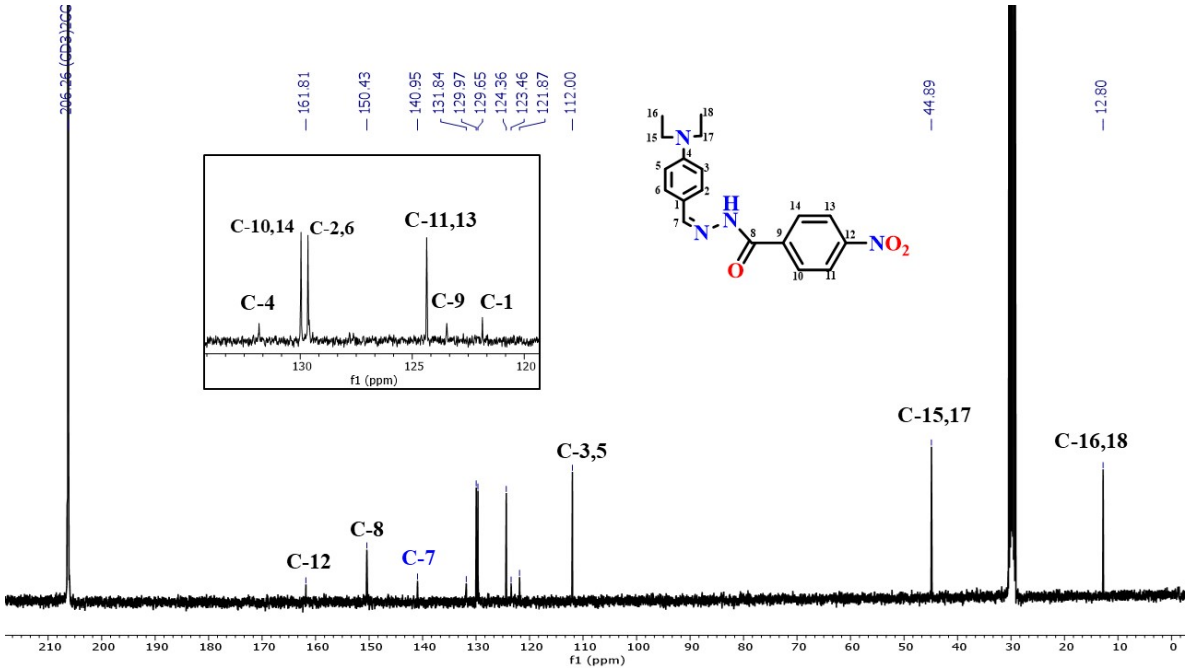

Figure S12. ^{13}C {1H} NMR Spectrum in acetone-d_6 of ligand **2**.

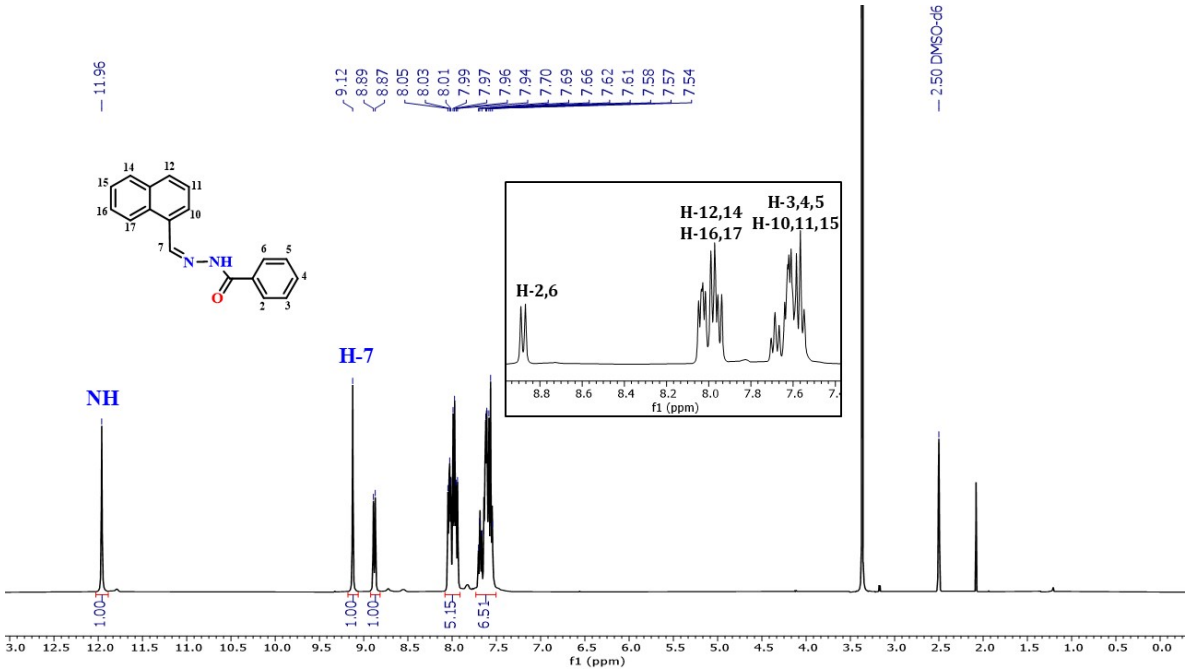

Figure S13. ^{1}H NMR Spectrum in DMSO-d_6 of ligand **3**.

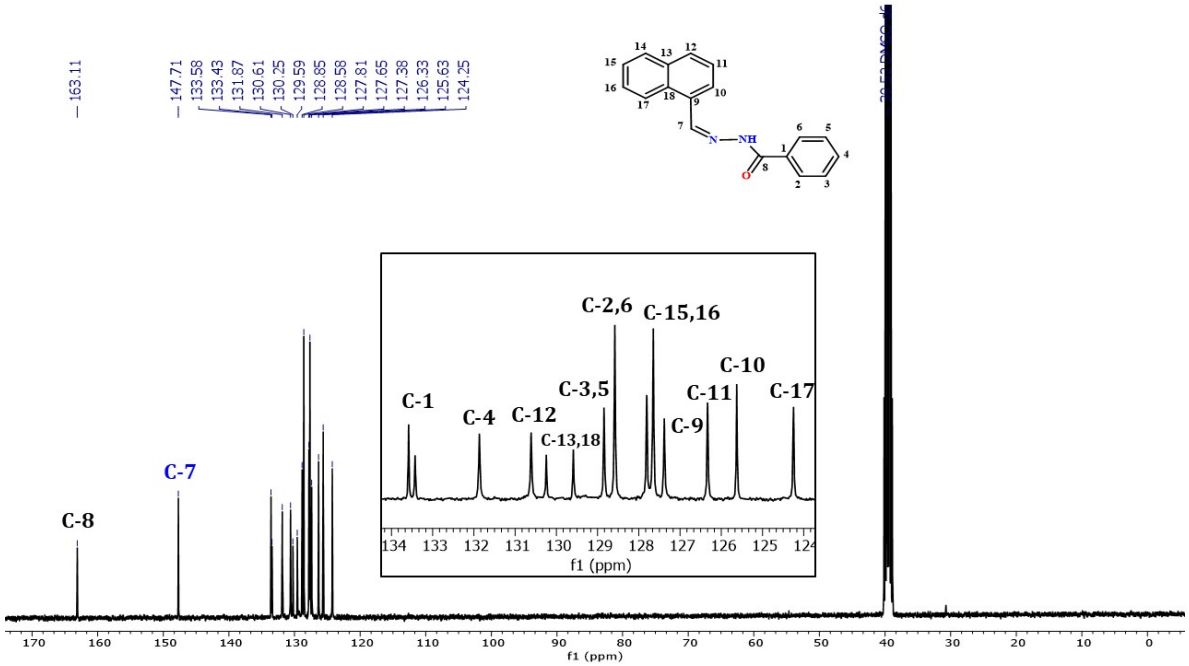

Figure S14. ^{13}C {1H} NMR Spectrum in DMSO-d_6 of ligand **3**.

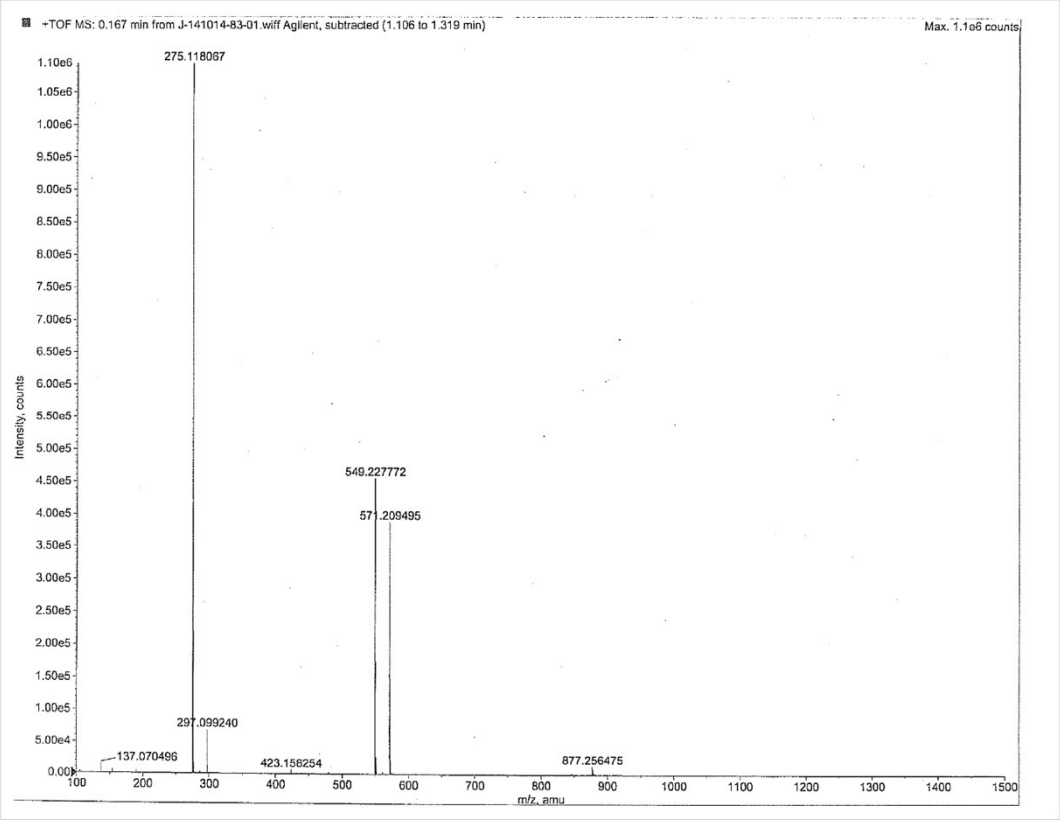

Figure S15. High resolution mass spectroscopy of ligand **3**, Chemical Formula: $C_{18}H_{15}N_2O$, Calculated *m/z*: 275.117889. Found 275.1180 (PPM error: 0.644536)

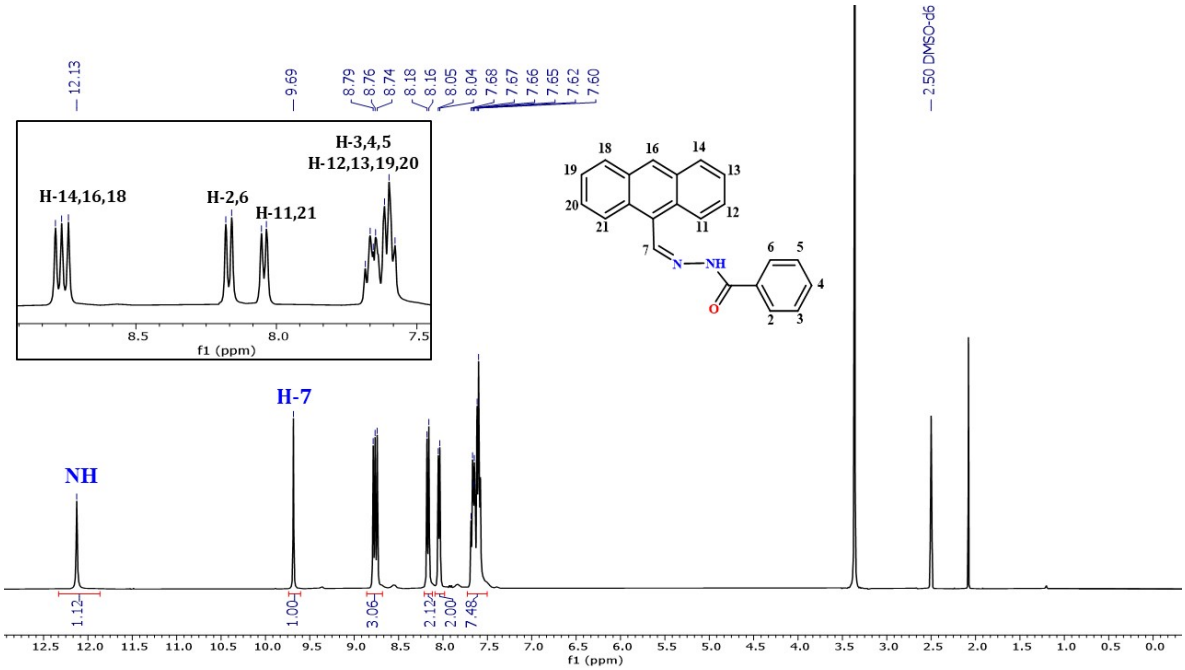

Figure S16. ^{1}H NMR Spectrum in DMSO-d_6 of ligand **4**.

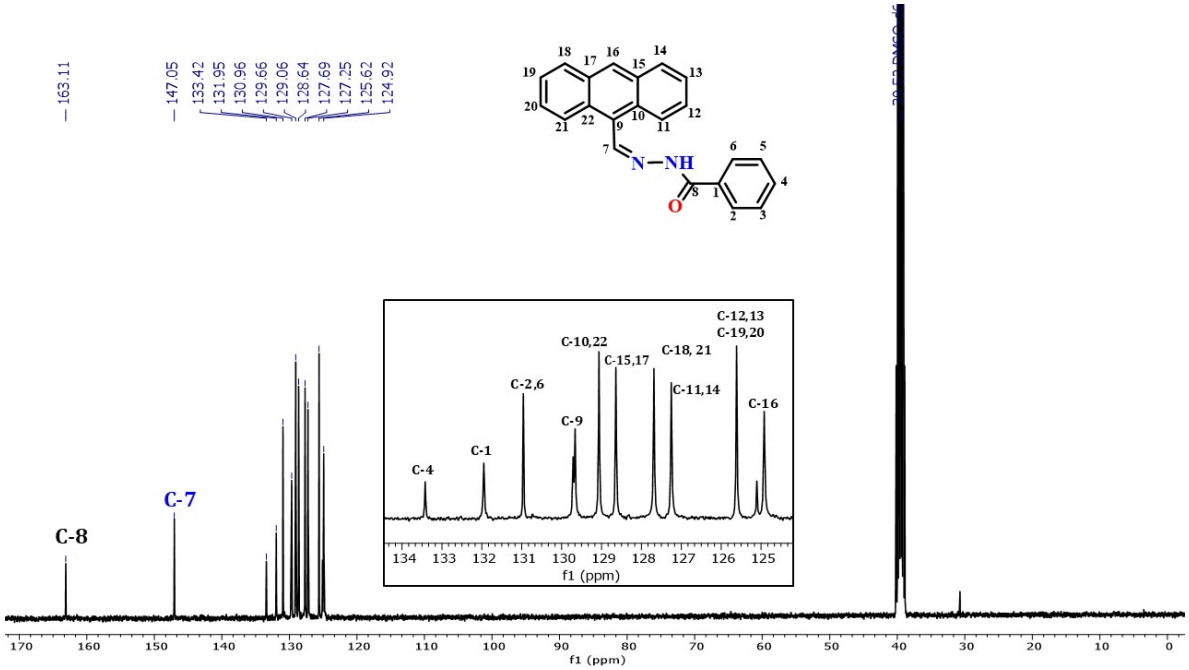

Figure S17. ^{13}C {1H} NMR Spectrum in DMSO-d_6 of ligand **4**.

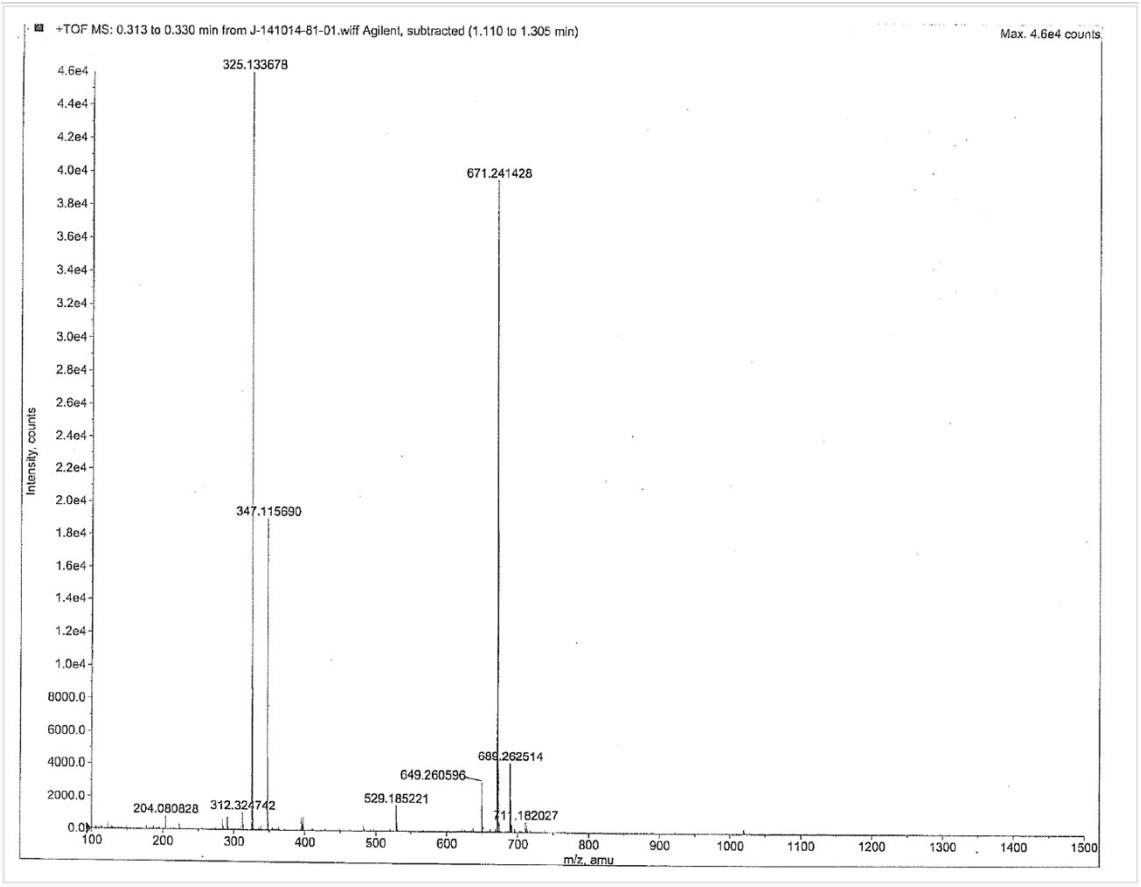

Figure S18. High resolution mass spectroscopy of ligand **4.** Chemical Formula: $C_{22}H_{17}N_2O$, Calculated *m/z*: 325.133539. Found 325.133678 (PPM error: 0.425190)

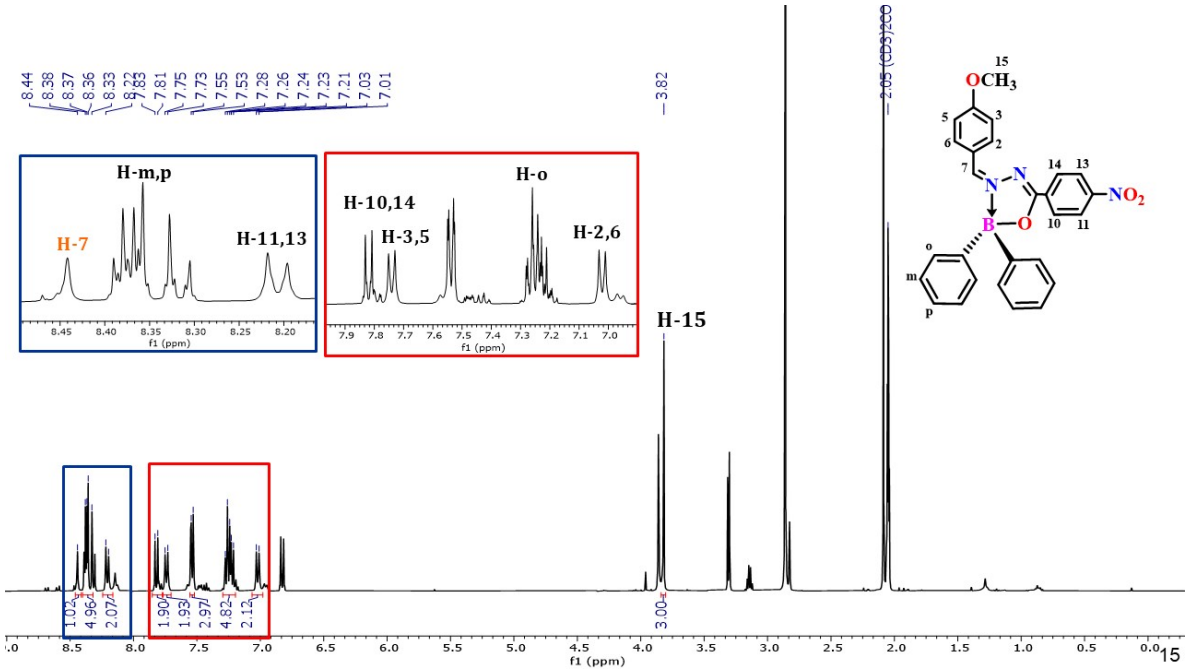

Figure S19. ^{1}H NMR Spectrum in acetone-d_6 of compound **5**.

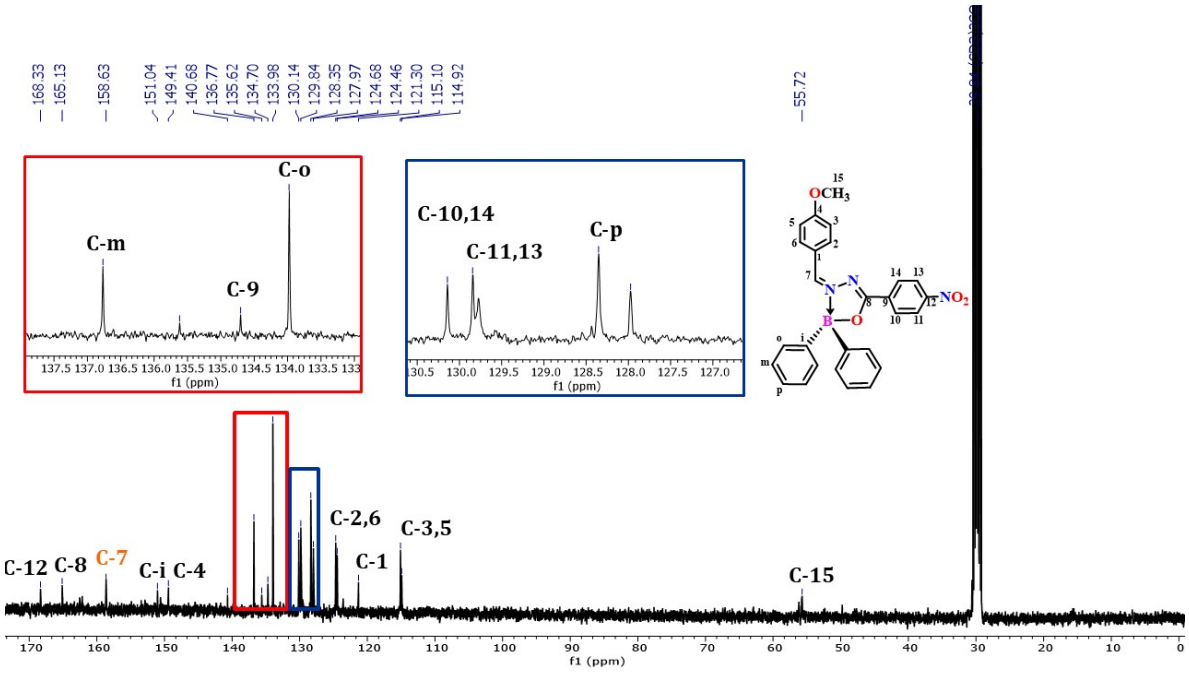

Figure S20. ^{13}C {1H} NMR Spectrum in Acetone-d_6 of compound **5.**

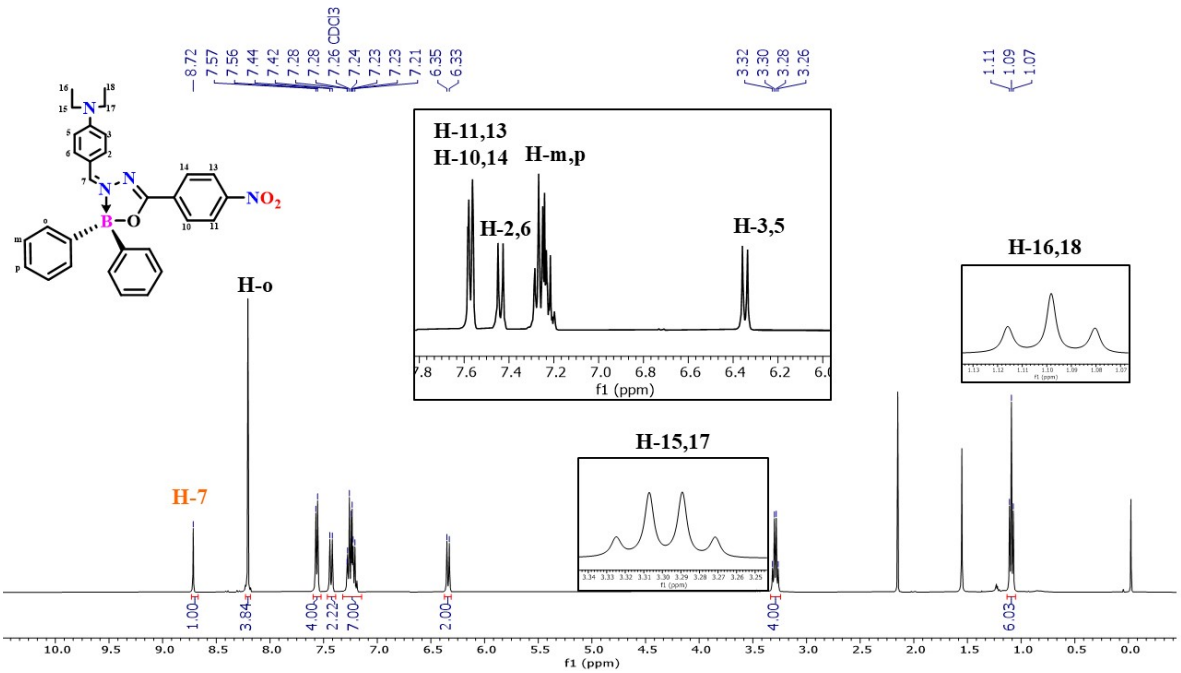

Figure S21. ^{1}H NMR Spectrum in $CDCl_3$ of compound **6**.

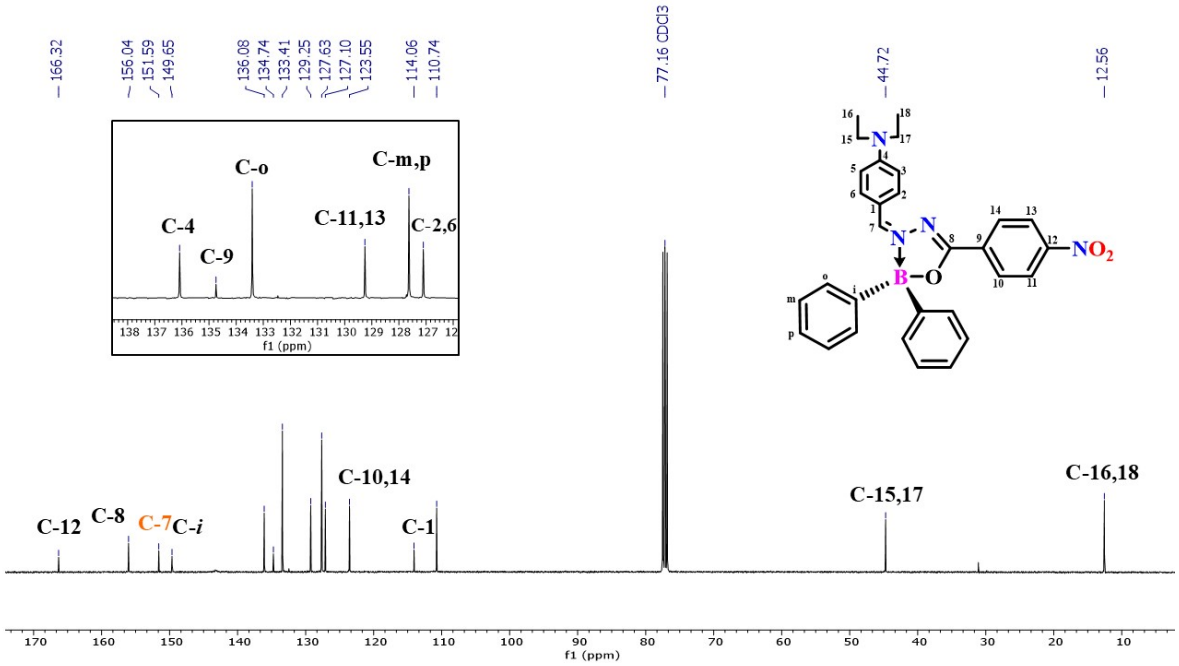

Figure S22. ^{13}C {1H} NMR Spectrum in $CDCl_3$ of compound **6**.

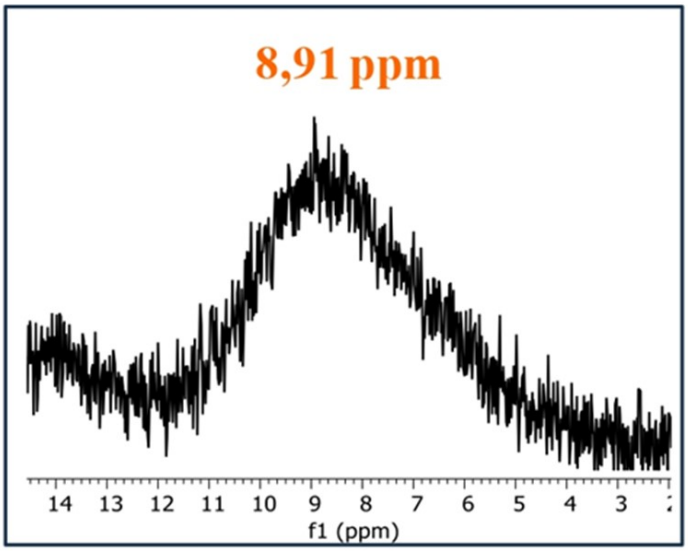

Figure S23. {1H} NMR Spectrum in $CDCl_3$ of compound **6**.

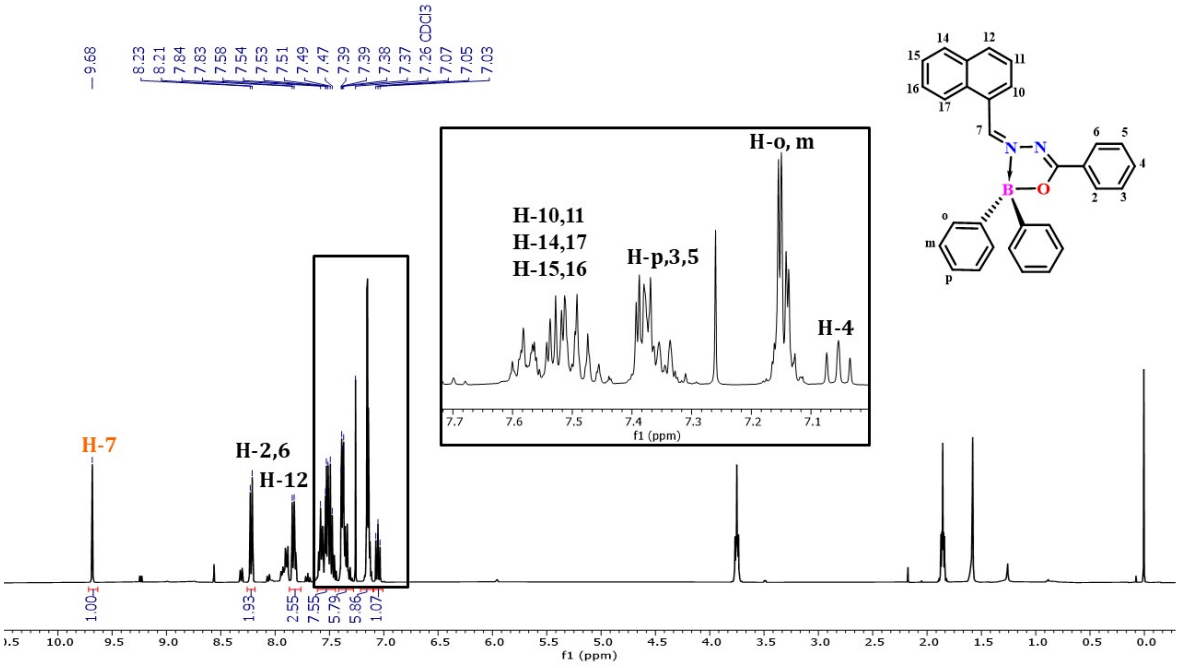

Figure S24. [1]H NMR Spectrum in $CDCl_3$ of compound **7**.

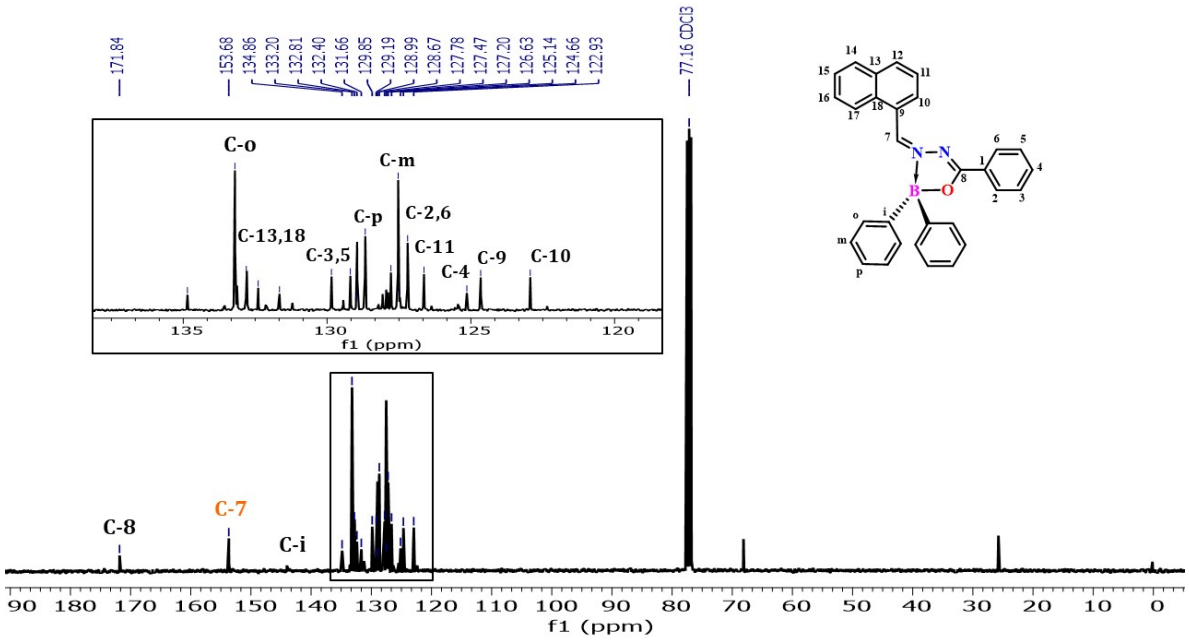

Figure S25. ^{13}C {1H} NMR Spectrum in $CDCl_3$ of compound **7**.

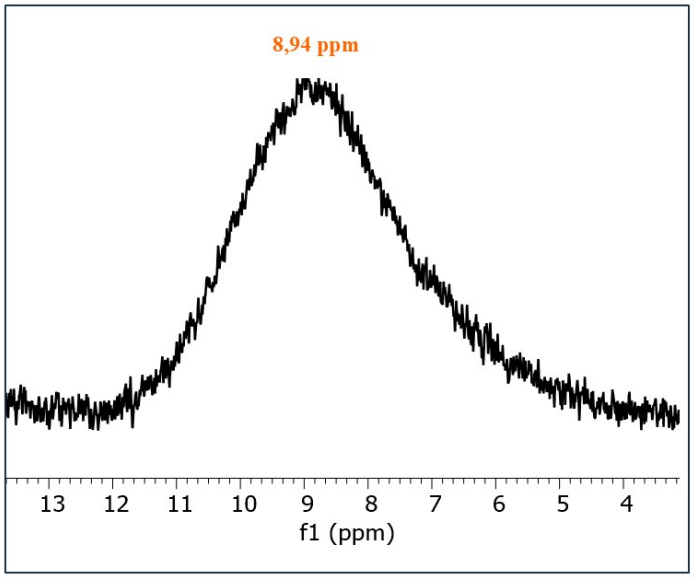

Figure S26. ^{11}B {1H} NMR Spectrum in $CDCl_3$ of compound **7**.

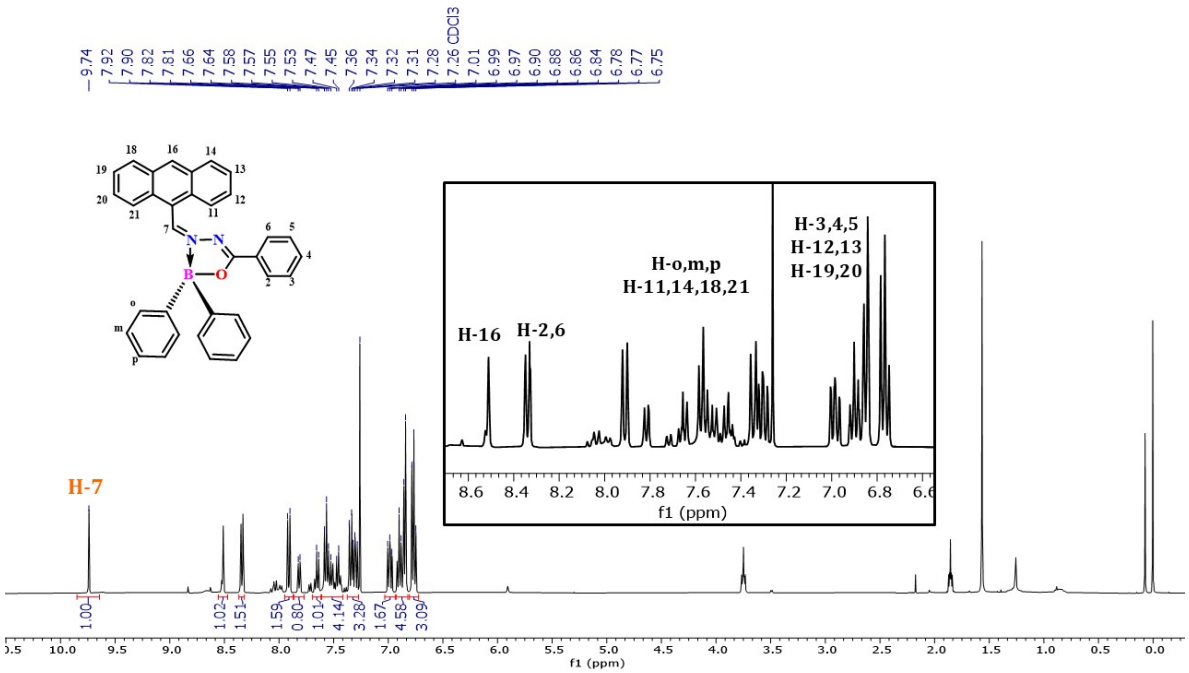

Figure S27. ^{1}H NMR Spectrum in $CDCl_3$ of compound **8**.

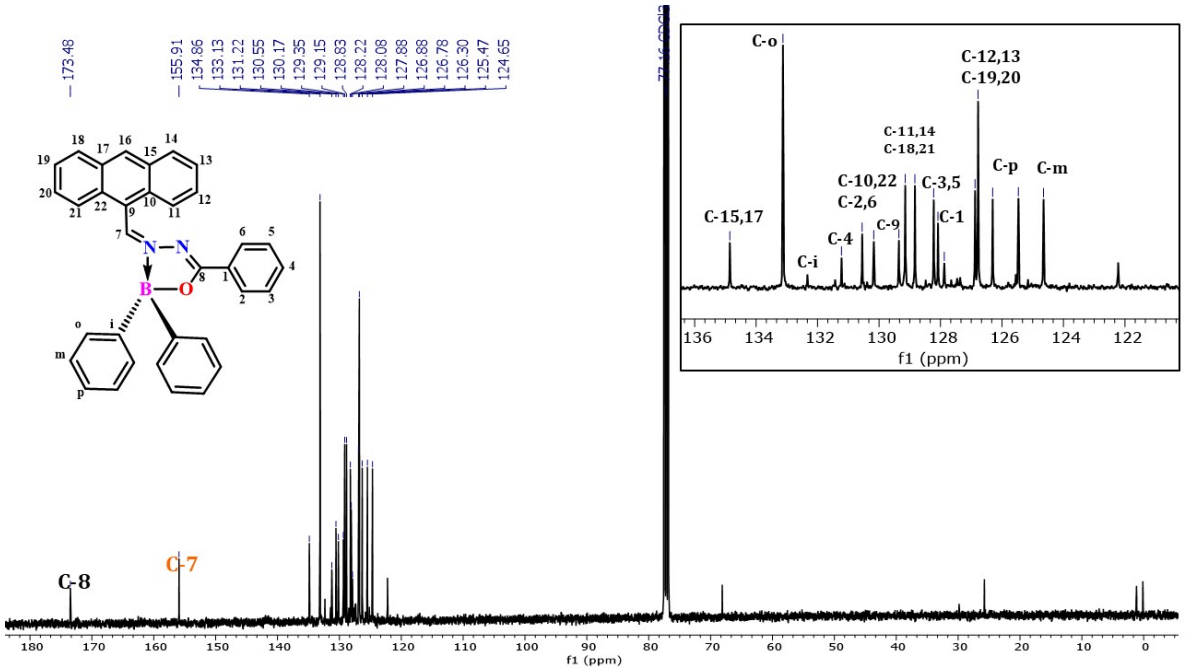

Figure S28. ^{13}C {1H} NMR Spectrum in $CDCl_3$ of compound **8**.

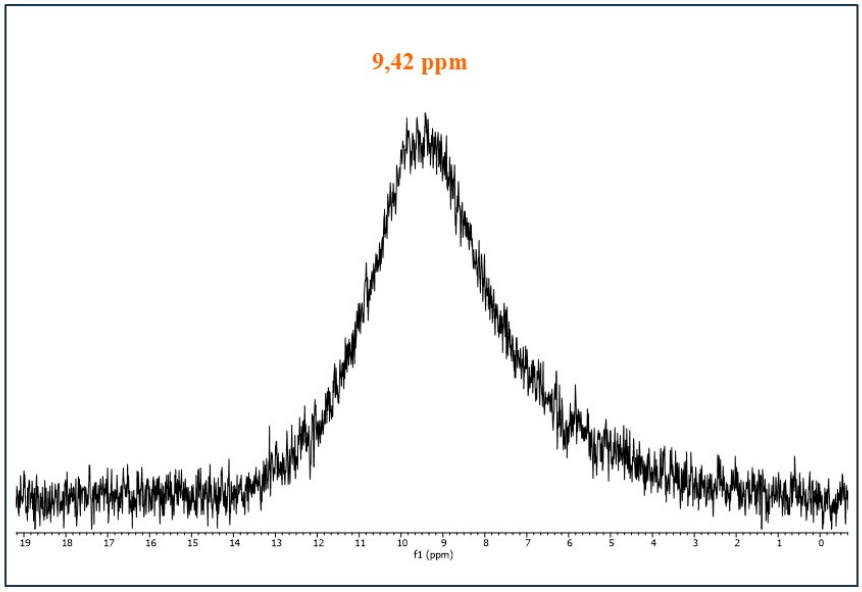

Figure S29. ^{11}B {1H} NMR Spectrum in $CDCl_3$ of compound **8**.

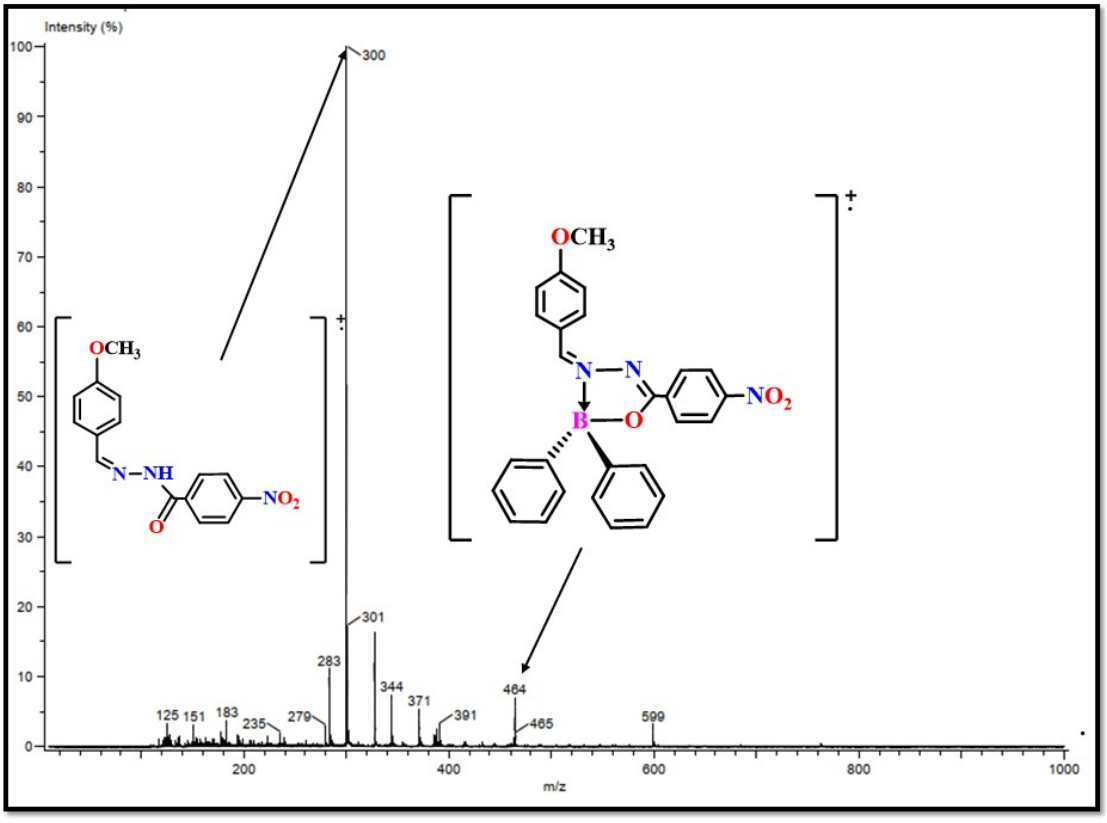

Figure S30. ESI-MS spectrum of compound **5**.

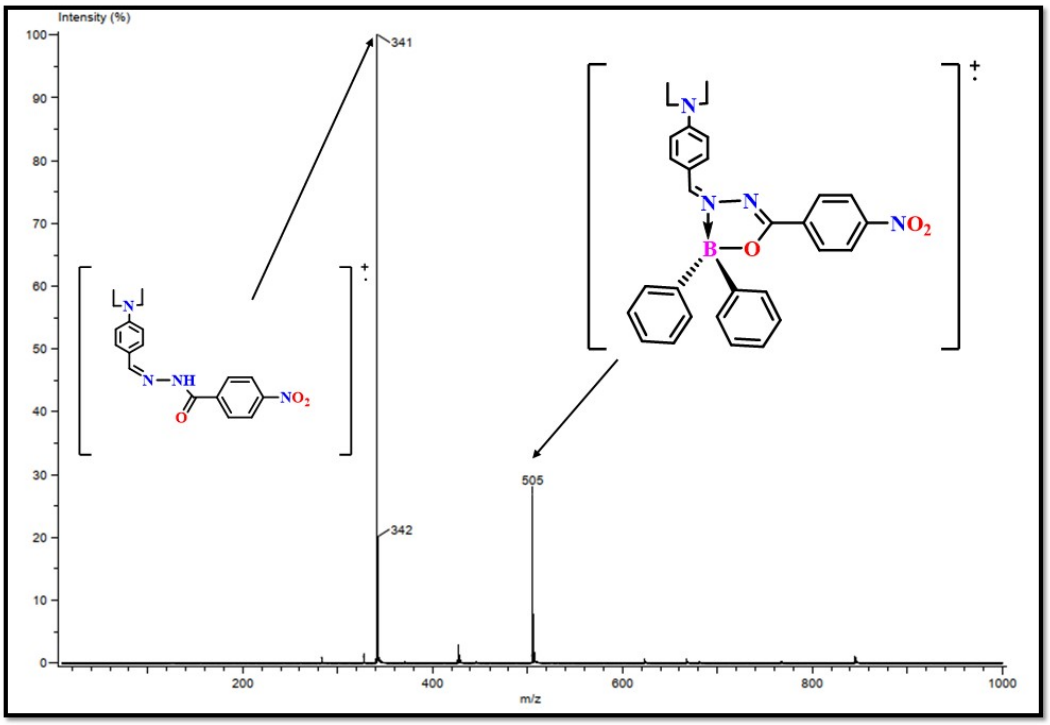

Figure S31. ESI-MS spectrum of compound **6**.

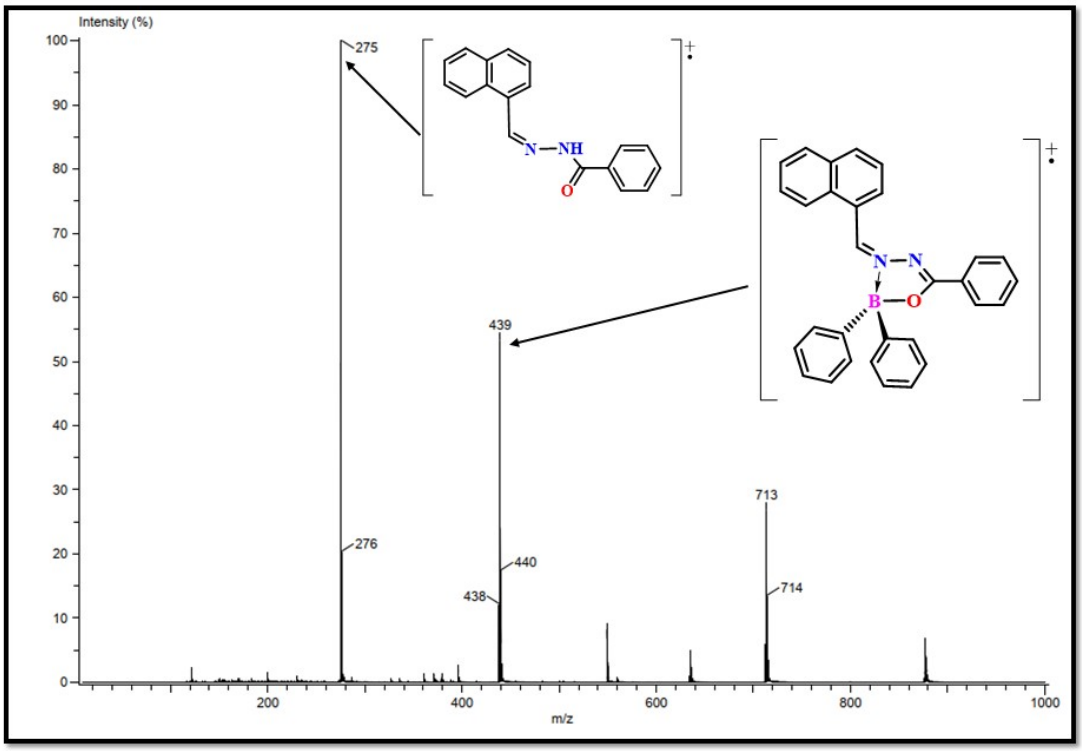

Figure S32. ESI-MS spectrum of compound **7**.

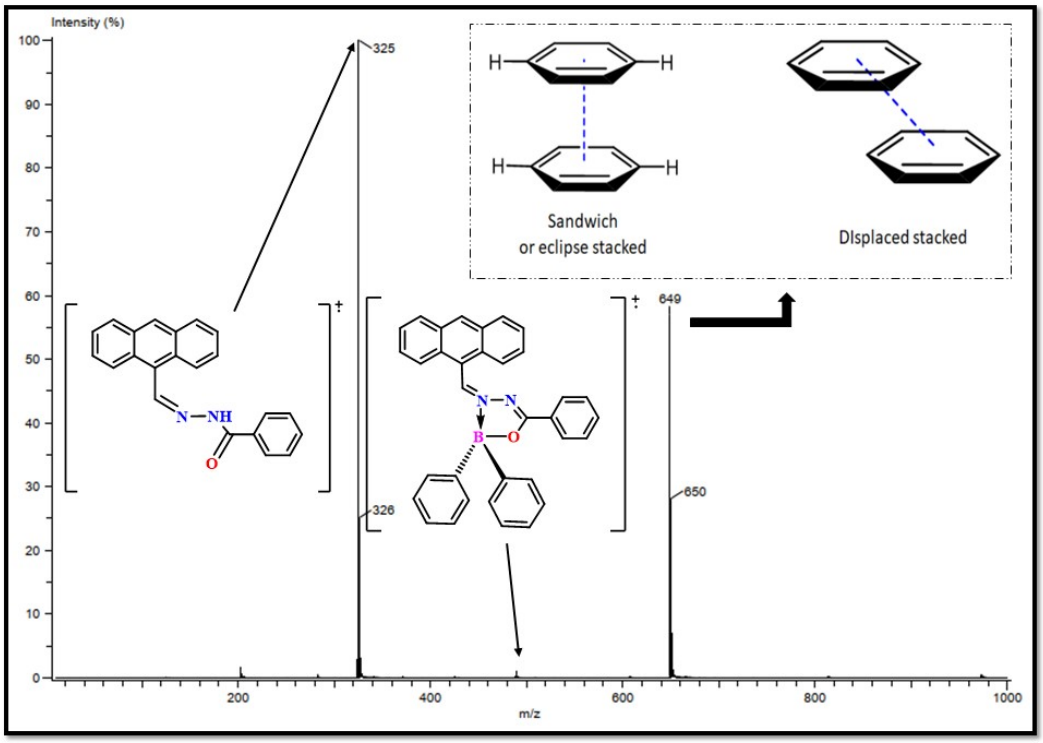

Figure S33. ESI-MS spectrum of compound **8**.

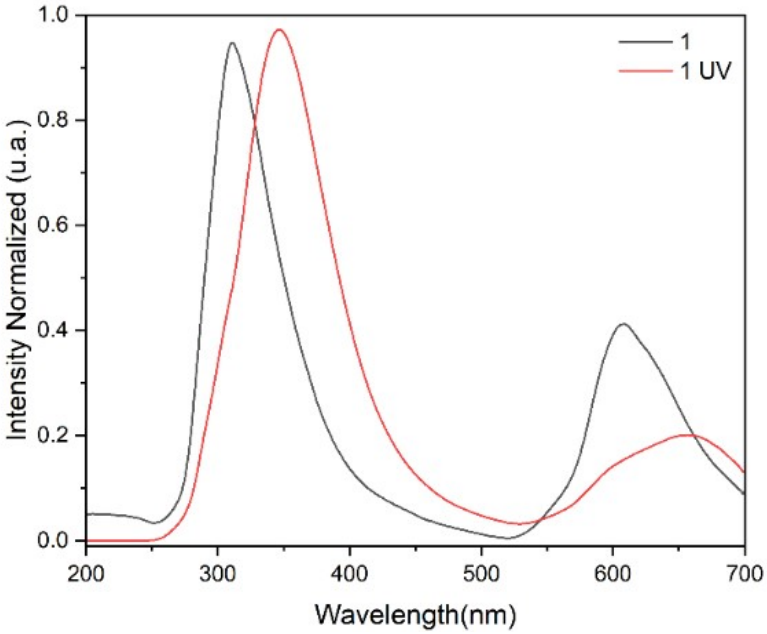

Figure S34. Emission spectra of **1**.

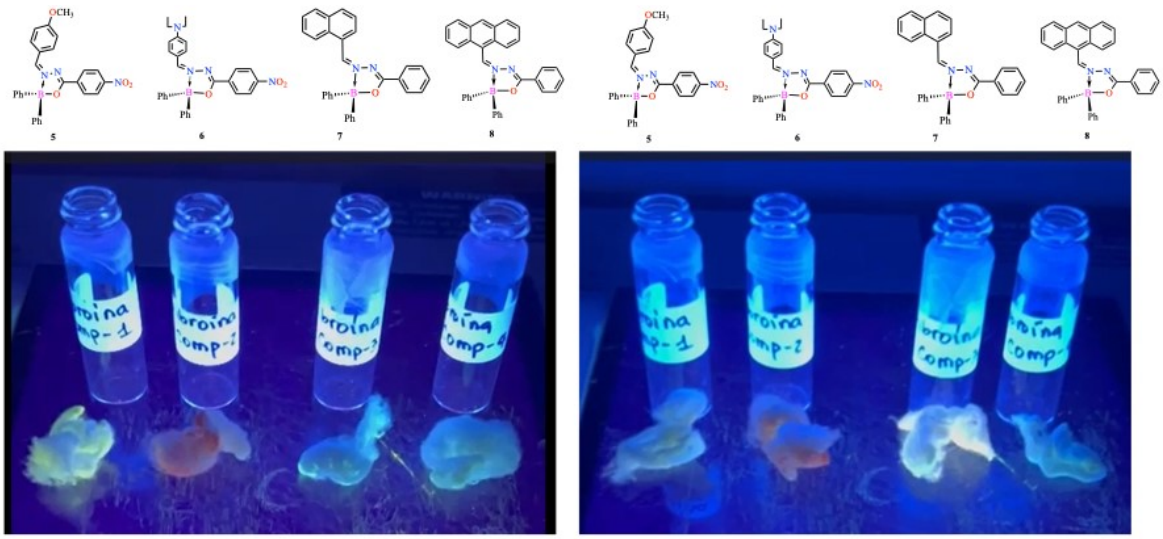

Figure S35. Pictures of fluorescent fibers pristine and after rubbing under UV ligth.

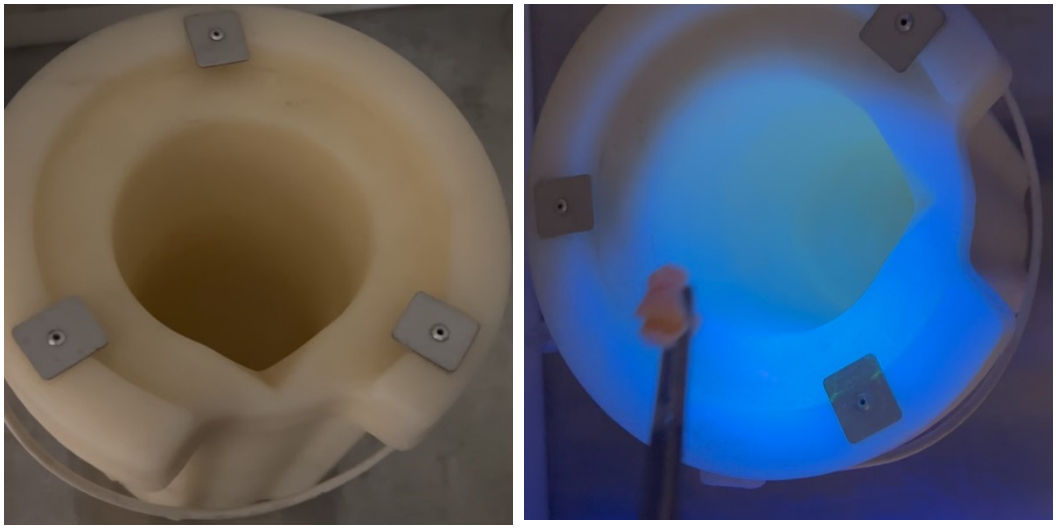

Figure S36: Video showing the fluorescent stained fiber was immersed in liquid nitrogen with compounds **5** (left) and **6** (right). Double-click to play.

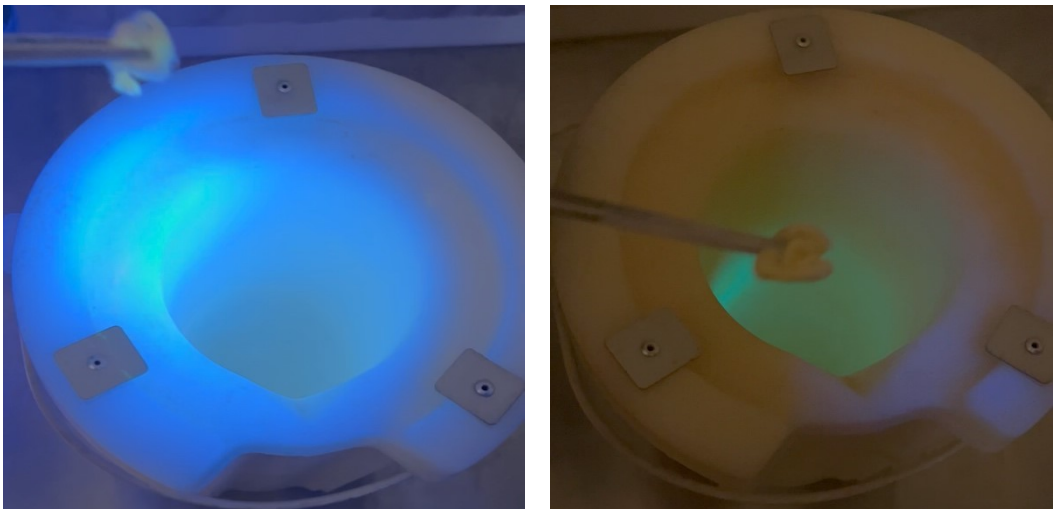

Figure S37: Video showing the fluorescent stained fiber was immersed in liquid nitrogen with compounds **7** (left) and **8** (right). Double-click to play.

Table S5. Crystal data for compound **5**

	5
Empirical formula	$C_{27}H_{22}BN_3O_4$
Formula weight (g/mol)	463,30
Crystal system	orthorhombic
Space group	$Pca2_1$
Temperature (K)	100(2)
a, (Å)	42,06(3)
b, (Å)	6,299(4)
c, (Å)	9,079(5)
α, (deg)	90
β, (deg)	90
γ, (deg)	90
Volume, ($Å^3$)	2405,7
Z	4
Crystal Size, mm^3	0,190 x 0,210 x 0,220
R_1,a wR_2b (I >2σ(I))	0.0595, 0.0502
R_1,a wR_2b (all data)	0.0969, 0.4895

Table S6. Selected bond distances (Å) and bond angles (°) of **5**

	5
Bond lengths	
B(1)-O(1)	1,5203(13)
B(1)-C(25)	1,5997(17)
B(1)-C(19)	1,5984(17)
B(1)-N(2)	1,6200(15)
N(1)−N(2)	1,3972 (12)
Bond angles	
O(1)-B(1)-C(19)	110,14(9)
O(1)-B(1)-C(25)	110,55(9)
C(25)-B(1)-C(19)	117,64(9)
O(1)-B(1)-N(2)	95,59(7)
C(19)-B(1)-N(2)	111,51(9)
C(25)-B(1)-N(2)	109,20(9)

Quantum Yield Calculation

We have calculated Quantum yield with respect to quinine sulphate (QS) in 0.1 M H_2SO_4, using the following formula.[1-2]

$$Q_S = Q_R\left(\frac{I_S}{I_R}\right)\left(\frac{A_R}{A_S}\right)\left(\frac{\eta_S}{\eta_R}\right)^2$$

Where,

Q_S = quantum yield of sample

Q_R = quantum yield of reference

I_S = area under PL curve of sample

I_R = area under PL curve of reference

A_R = absorbance of the reference

A_S =absorbance of the sample

η_S = refractive index of sample

η_R = refractive index of reference.

Q.Y. of quinine sulphate = 0.54; Refractive Index: water = 1.33 (The concentration of all samples and the reference quinine sulphate were adjusted so that the optical densities of all samples were 0.020 ± 0.003 at the excitation wavelength (365 nm)).

1.- Q. Zhang, Y. Gao, S. Zhang, J. Wu, H. Zhou, J. Yang, X. Tao, Y. Tian, *Dalton Trans*, **2012**, 41, 7067.
2.- J. E. Murphy, M. C. Beard, A. G. Norman, S. P. Ahrenkiel, J. C. Johnson, P. Yu, O. I. Micic, R. J. Ellingson, A. J. Nozik, *J. Am. Chem. Soc*, **2006**, 128, 3241