Synthesis, Structure, Spectral and Electrochemical Properties of New Visible to NIR Absorbing 3-Pyrrolyl BODIPY Derivatives

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Supporting information

Content

MATERIALS AND METHODS

Materials: The chemicals were obtained from reliable vendors like Merck and TCI. These suppliers supplied $BF_3.OEt_2$, 2, 3-dichloro-5, 6-dicyano-1, 4-benzoquinone (DDQ), trifluoroacetic acid (TFA), 4-amino-1,2,4-triazole, 2-aminothiazole, 2-amino benzithiazole, phenylhydrazine, 2-aminothiophenol, and malononitrile so on. All other compounds used in the synthesis were of reagent grade quality unless specified differently. To ensure the purity and separation of chemicals throughout the purification process, column chromatography was carried out using silica gel (100-200 mesh) and basic alumina.

Methods:

- All the ^{1}H and ^{13}C NMR spectra were recorded in $CDCl_3$ on Bruker 400 and 500 MHz instruments. The frequencies for the ^{13}C nucleus are 100.06 and 125.77 MHz for 400 and 500 MHz instruments, respectively. Similarly, the frequencies for the ^{11}B and ^{19}F nucleus are 193 and 376 MHz for 400 MHz instruments.
- Absorption spectra were obtained with a UV 3600 Shimadzu. Steady-state fluorescence spectra were obtained with Horiba FluoroMax 4 spectrometer.
- Single crystals of compound **3**, **8,** and **8-Re(I)** were picked up with nylon loops and were mounted on Bruker Bruker APEX-II CCD diffractometer equipped with a Mo-target rotating-anode X-ray source and a graphite monochromator (Mo-Kα, λ = 0.71073 Å). The crystal was maintained at a temperature of 150 K during data collection. The structure was solved by direct methods and subsequent difference Fourier techniques. Low angle, poor intensity diffraction and twin nature of single crystal resulted slightly higher R1 and wR2 value than normal range for all the compound. The structures were solved using the Olex2 Solve 1.5 program (Bourhis et al., 2015) with dual-space methods, employing Olex2 1.5-dev (Dolomanov et al., 2009) as the graphical interface. The model was refined using olex2.refine 1.5-dev (Bourhis et al., 2015) with full matrix least squares minimization on F^2. All the crystal parameter of 8 are given in Table S1. All the relevant bond angle and bond distance parameters are given in Table S2 in the supporting information file.
- Studies on cyclic voltammetry (CV) were conducted using the BAS electrochemical system, employing a three-electrode configuration: platinum wire for the auxiliary electrode, saturated calomel for the reference electrode, and glassy carbon for the

working electrode. As a supporting electrolyte, tetrabutylammonium perchlorate was used in the dry dichloromethane studies.

- The HR and LR mass spectra were recorded with a Q-Tof micro mass spectrometer and an Agilent advance bio 6545XT LC/Q-TOF instrument.
- Fluorescence quantum yields were determined in each case by comparing the corrected spectrum with that of Rhodamine 6G (Φ =0.95) in EtOH by taking the area under total emission using the procedure reported earlier.[S1- S2]
- The exponential decay curve of compounds was fitted appropriately with a mono/biexponential equation. The average lifetime (τ_{av}) was calculated following the equations depicted in the literature.[S3]
- DFT was used in a Gaussian 09W program package to perform quantum chemistry calculations (gas phase/vacuum) for ground state energy minimized structures for compounds **3-8** and **8-Re(I)**. The density functional theory (DFT) method, hybrid functional B3LYP in conjunction with the basis set 6-31G(d,p) helped in optimizing the structures of compounds **3-8** and LANL2DZ for **8-Re(I)** complex.[S4-S5] The oscillator strengths were determined using the same basis and functional hybrid set, whereas the vertical excitation energies were determined with the use of TD-DFT methods. In the toluene media, all calculations were performed utilizing the Self-Consistent Reaction Field (SCRF) under the Polarisable Continuum Model (PCM). Based on the optimized structures, TD-DFT with PCM model was used to extensively analyze the oscillator strengths and electronic absorption spectra.[S6-S7]

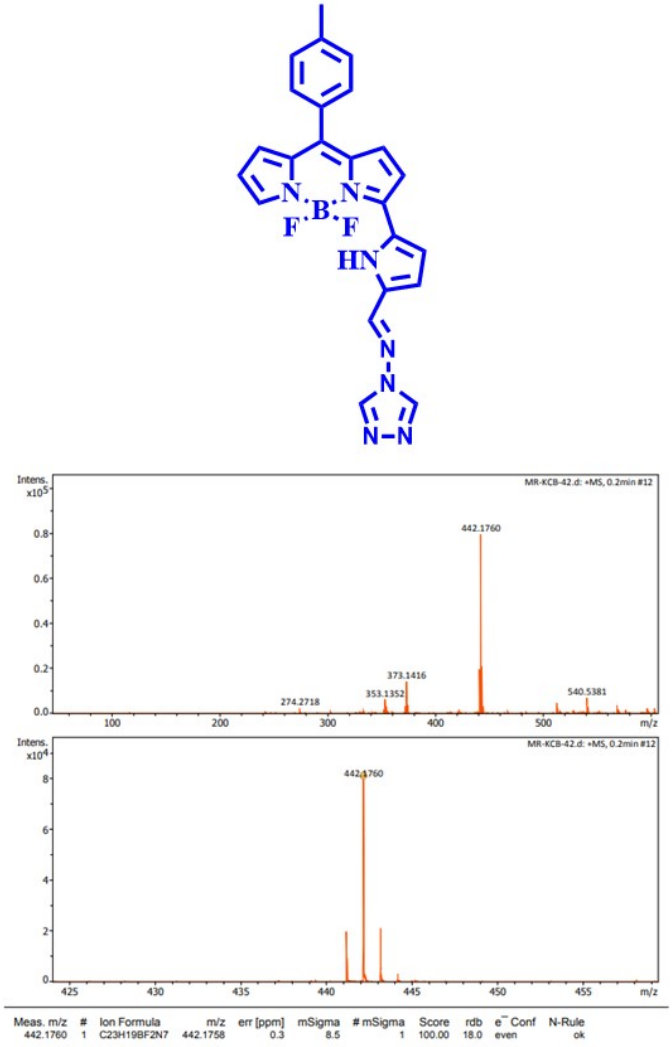


Figure S1. HR mass spectrum of the compound **3**.

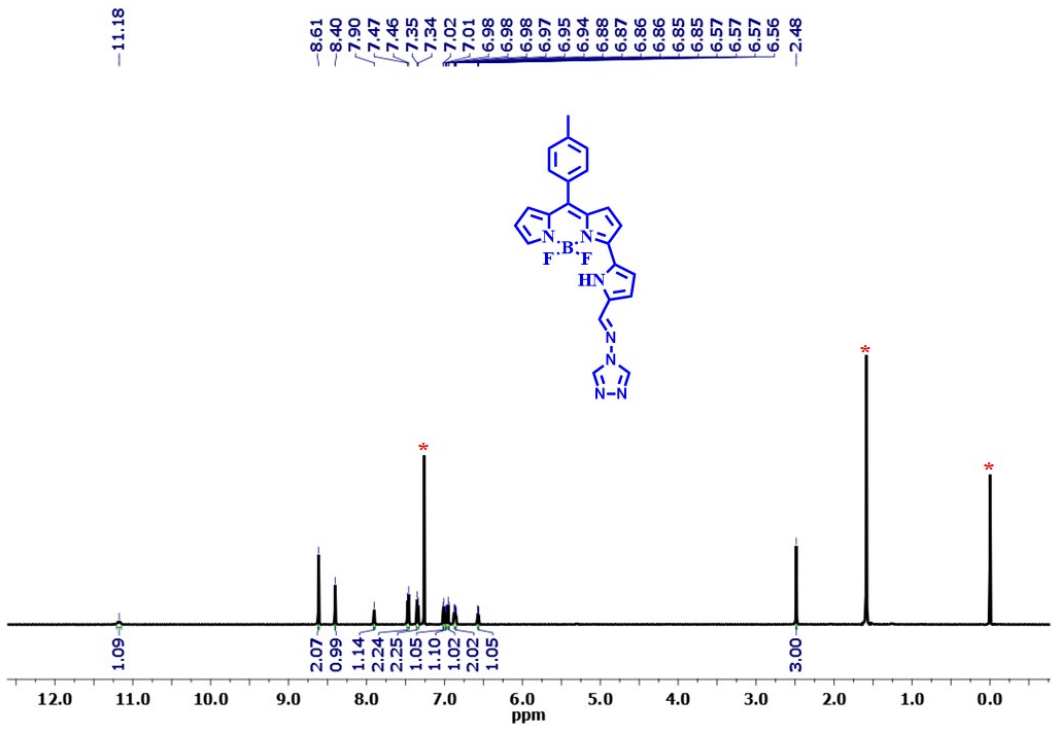


Figure S2. ^{1}H NMR spectrum of the compound **3** recorded in $CDCl_3$ at 25 °C; Note: Peaks marked with asterisk (*) are due to residual solvents.

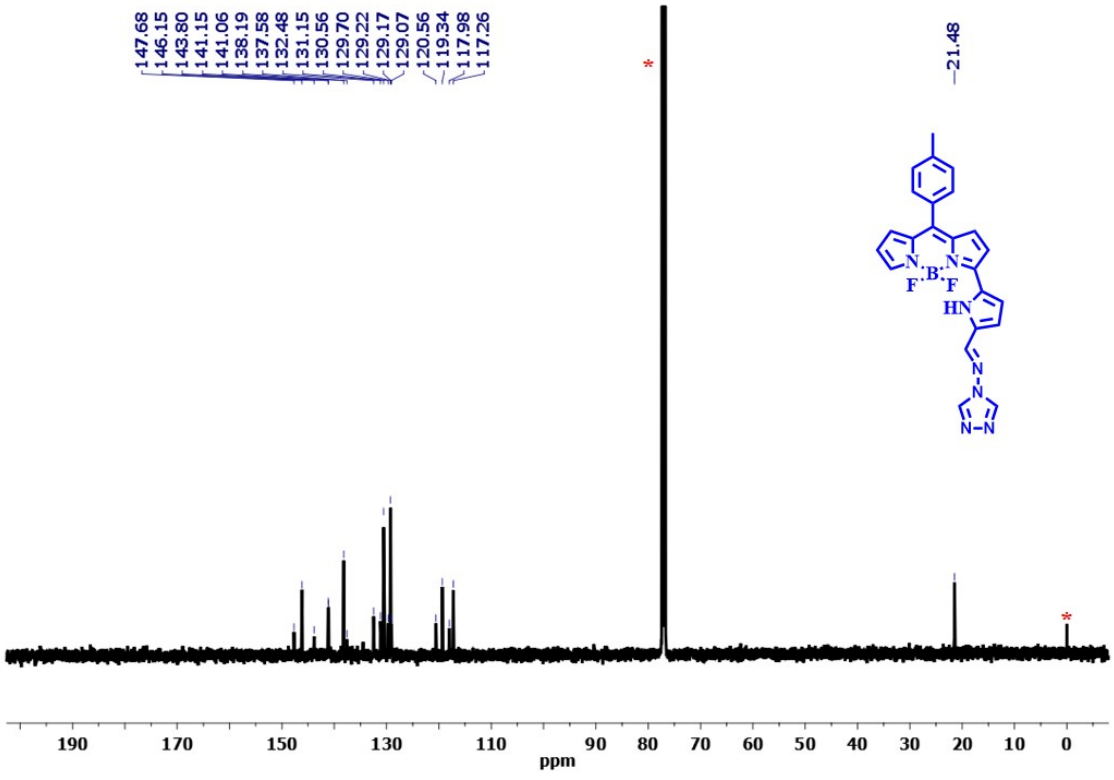


Figure S3. ^{13}C NMR spectrum of the compound **3** recorded in $CDCl_3$. Note: Peaks marked with asterisk (*) are due to residual solvents.

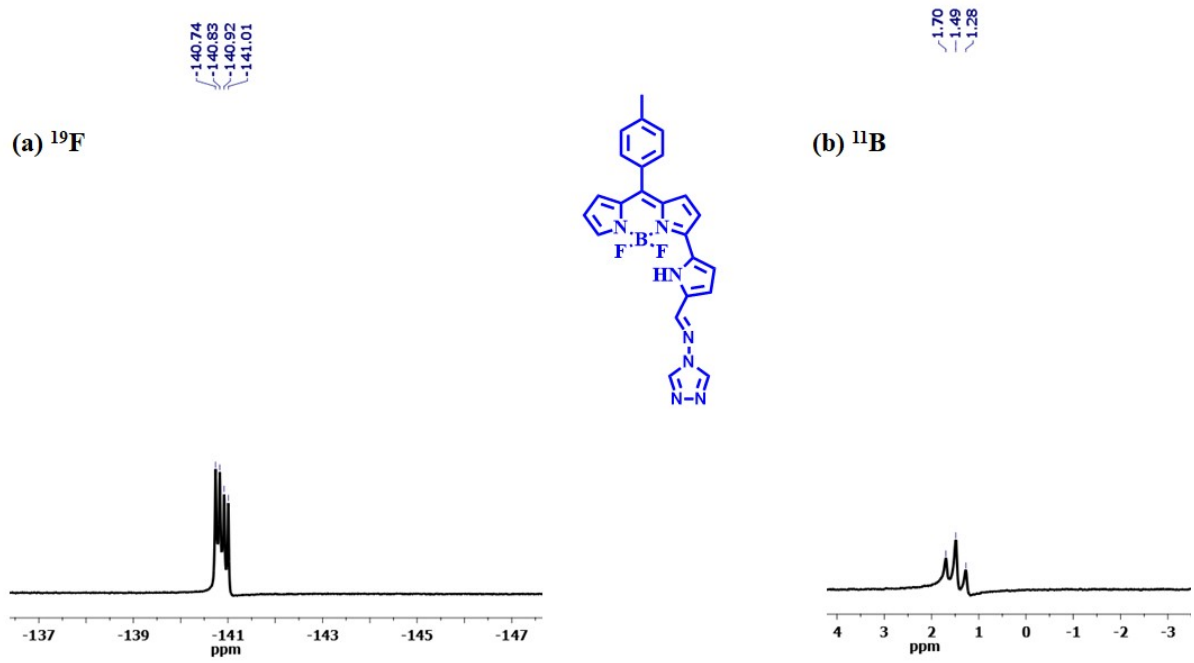


Figure S4. (a) ^{19}F and (b) ^{11}B NMR spectra of the compound **3** recorded in $CDCl_3$.

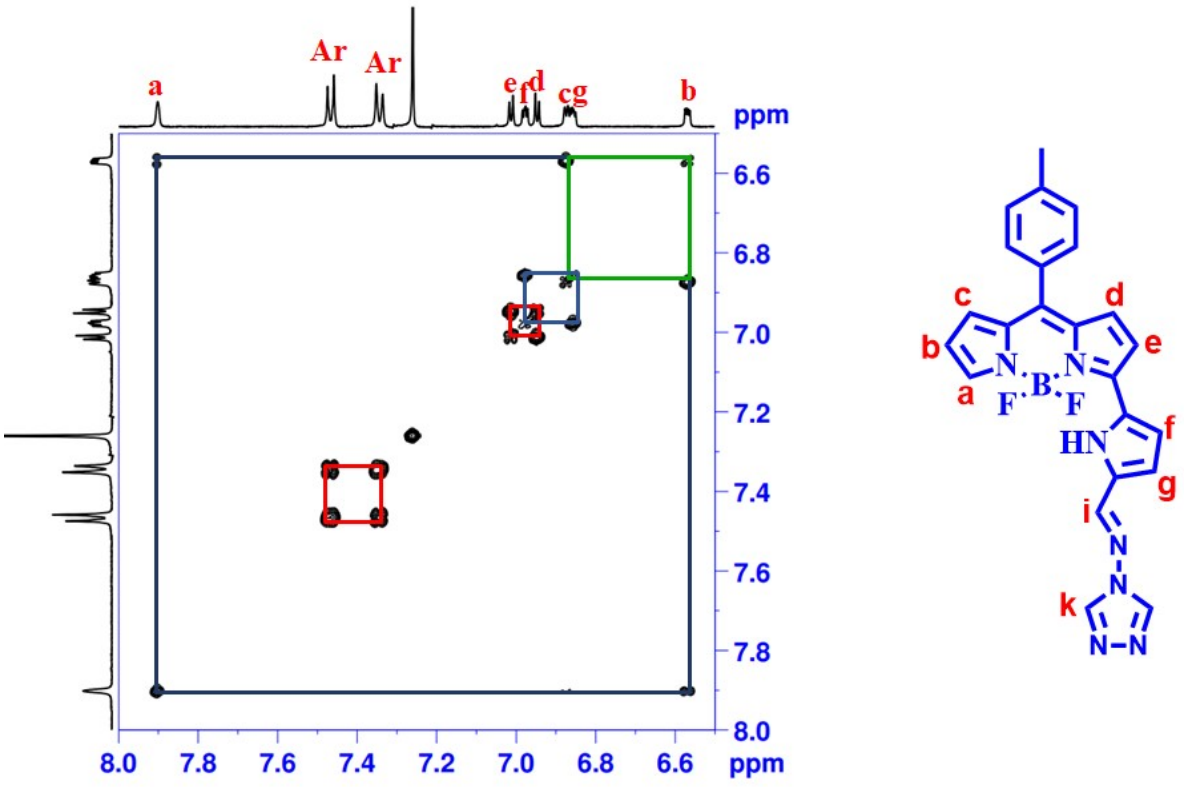


Figure S5. Partial ^{1}H-^{1}H COSY spectrum of the compound **3** in $CDCl_3$ at 25 ˚C.

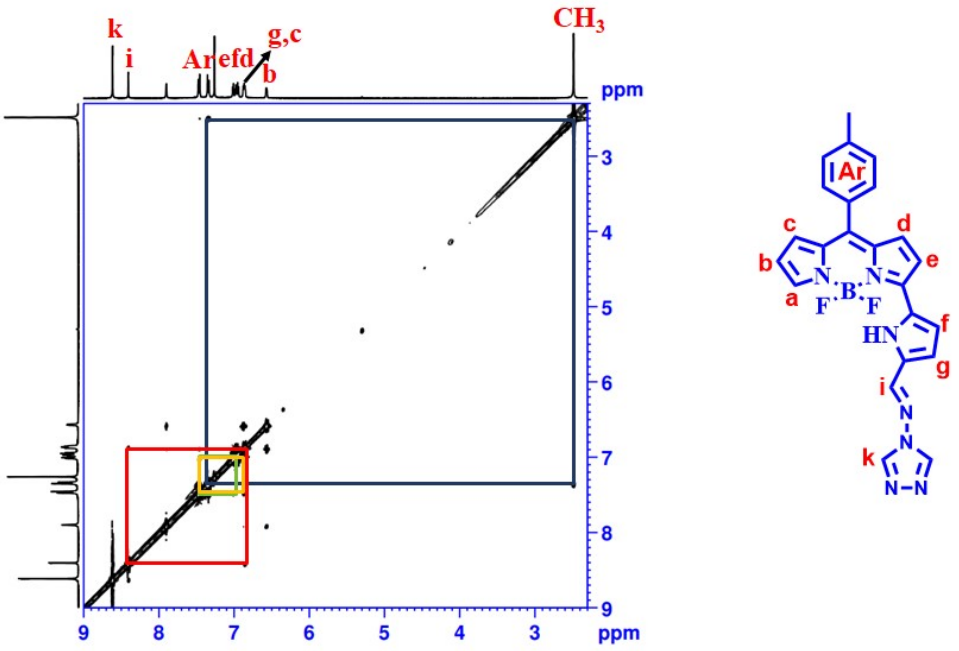


Figure S6. Partial ^{1}H-^{1}H NOESY spectrum of the compound **3** in $CDCl_3$ at 25 ˚C.

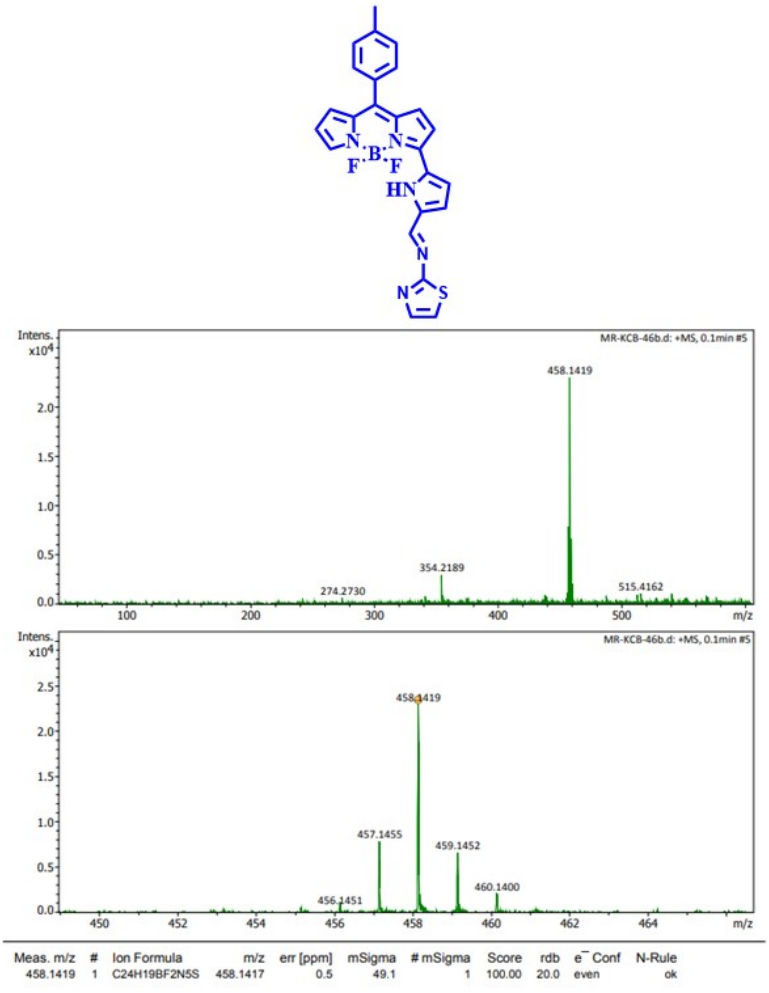


Figure S7. HR mass spectrum of the compound **4**.

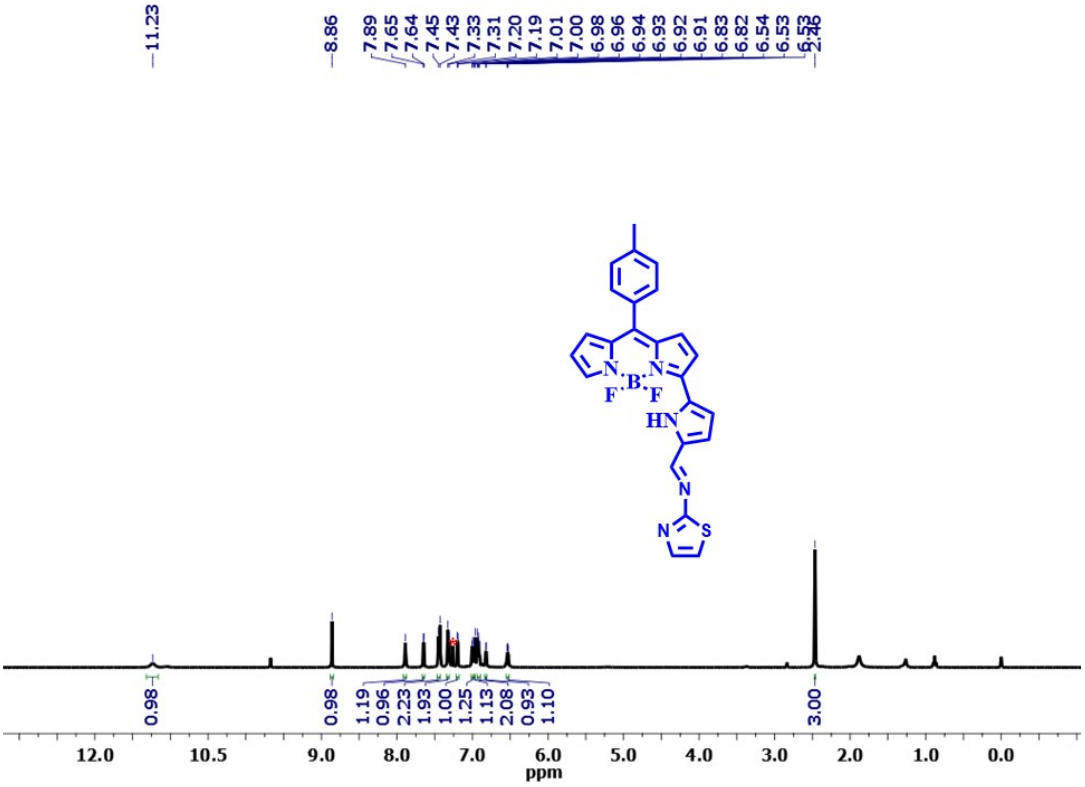


Figure S8. ^{1}H NMR spectrum of the compound **4** recorded in $CDCl_3$ at 25 °C; Note: Peaks marked with asterisk (*) are due to residual solvents.

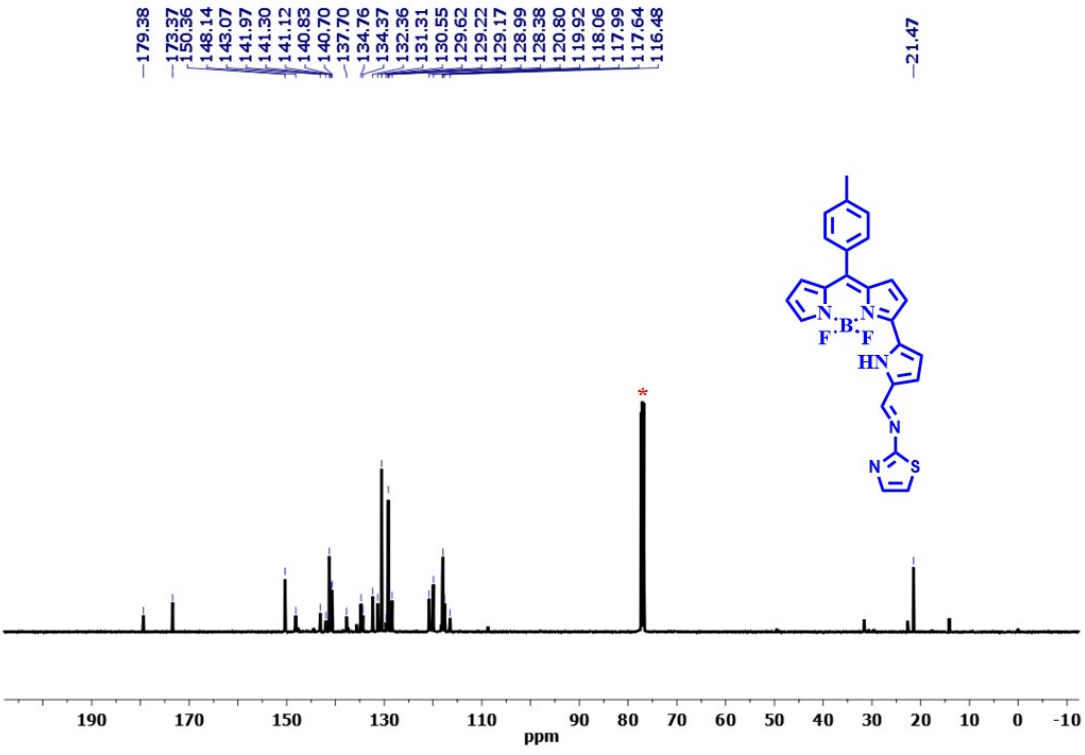


Figure S9. ^{13}C NMR spectrum of the compound **4** recorded in $CDCl_3$.

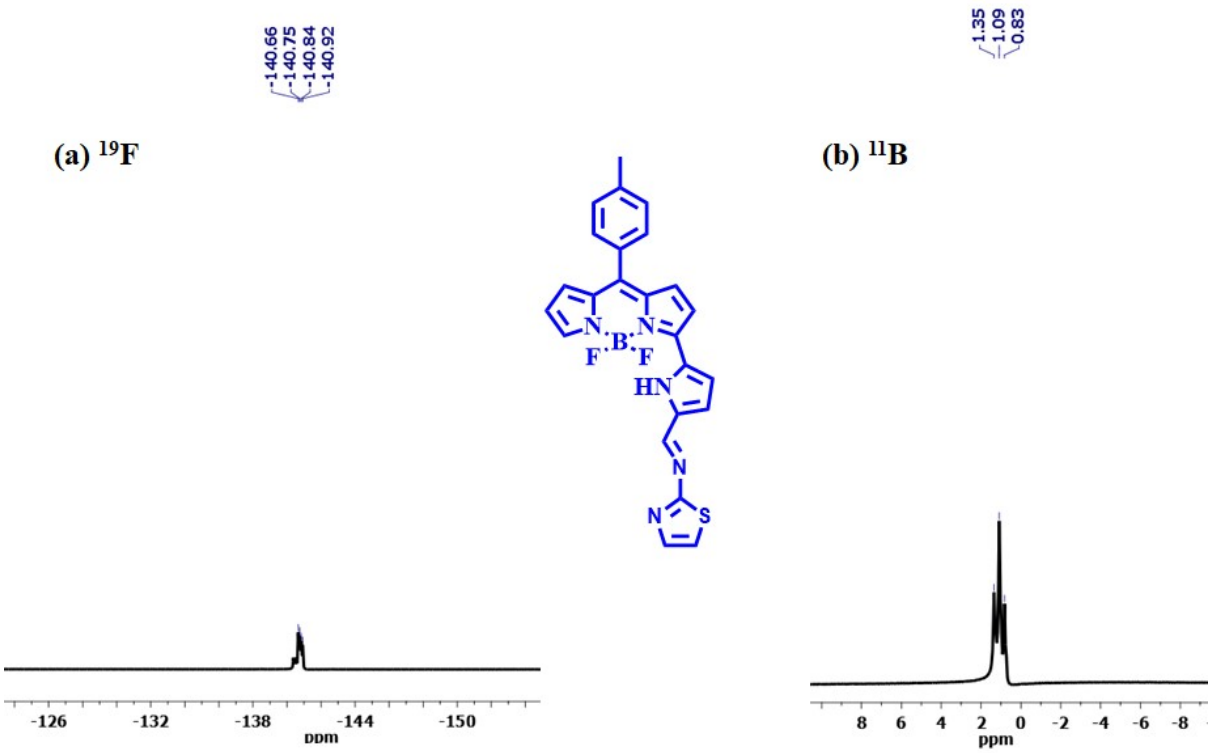


Figure S10. (a) ^{19}F and (b) ^{11}B NMR spectra of the compound **4** recorded in $CDCl_3$.

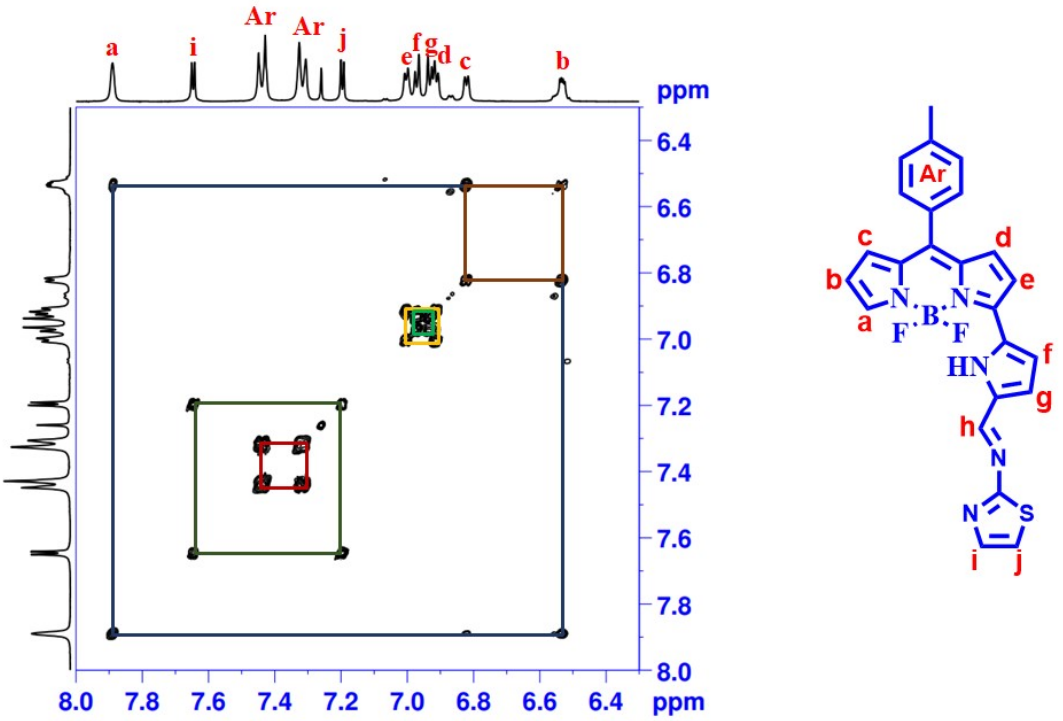


Figure S11. Partial ^{1}H-^{1}H COSY spectrum of the compound **4** in $CDCl_3$ at 25 ˚C.

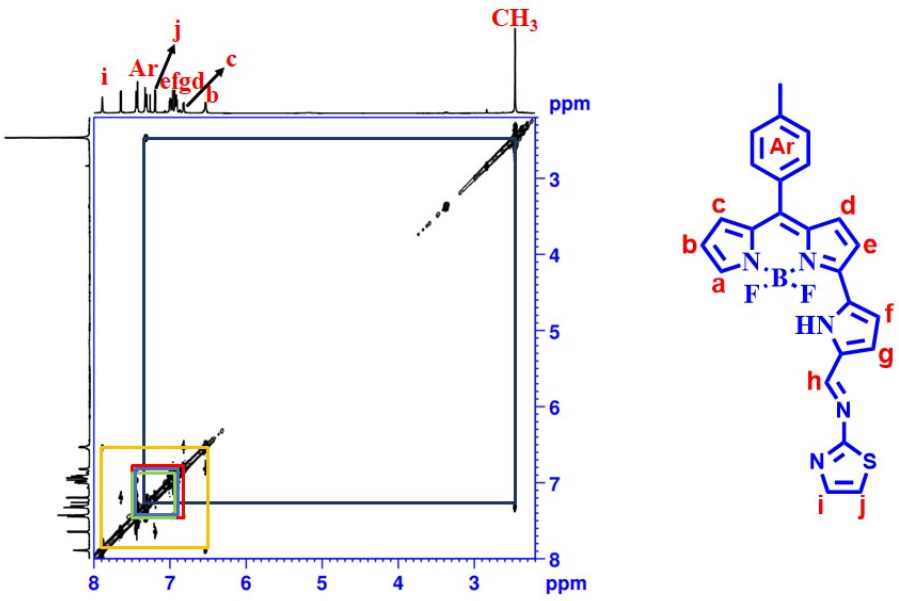


Figure S12. Partial ^{1}H-^{1}H NOESY spectrum of the compound **4** in $CDCl_3$ at 25 ˚C.

Compound Details

Cpd. 1: C28 H20 B F2 N5 S

Formula	m/z	Observed M/Z	Difference_Da	Difference_PPM	Score
C28 H20 B F2 N5 S	508.1586	508.158607151064	0.981881056816292	1.93988720441812	97.36

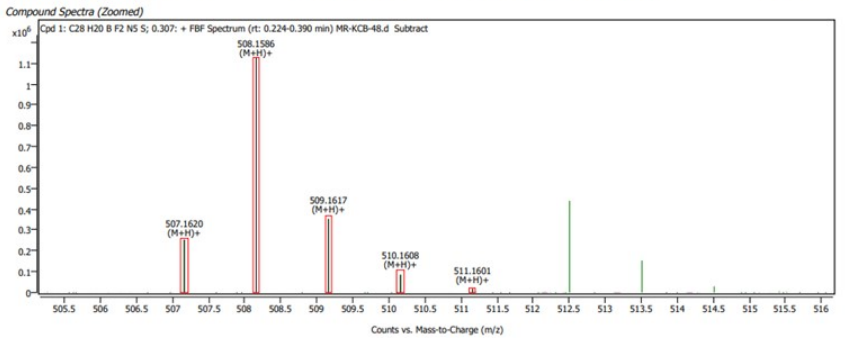


Figure S13. HR mass spectrum of the compound **5**.

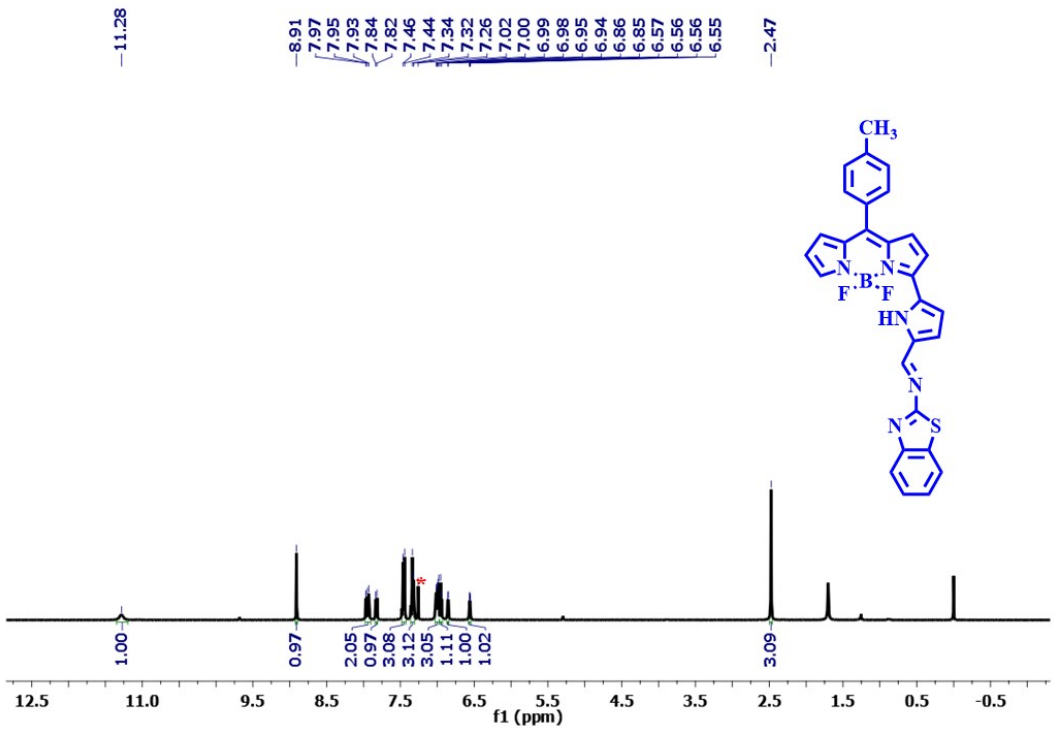


Figure S14. ^{1}H NMR spectrum of the compound **5** recorded in $CDCl_3$ at 25 ℃; Note: Peaks marked with asterisk (*) are due to residual solvents.

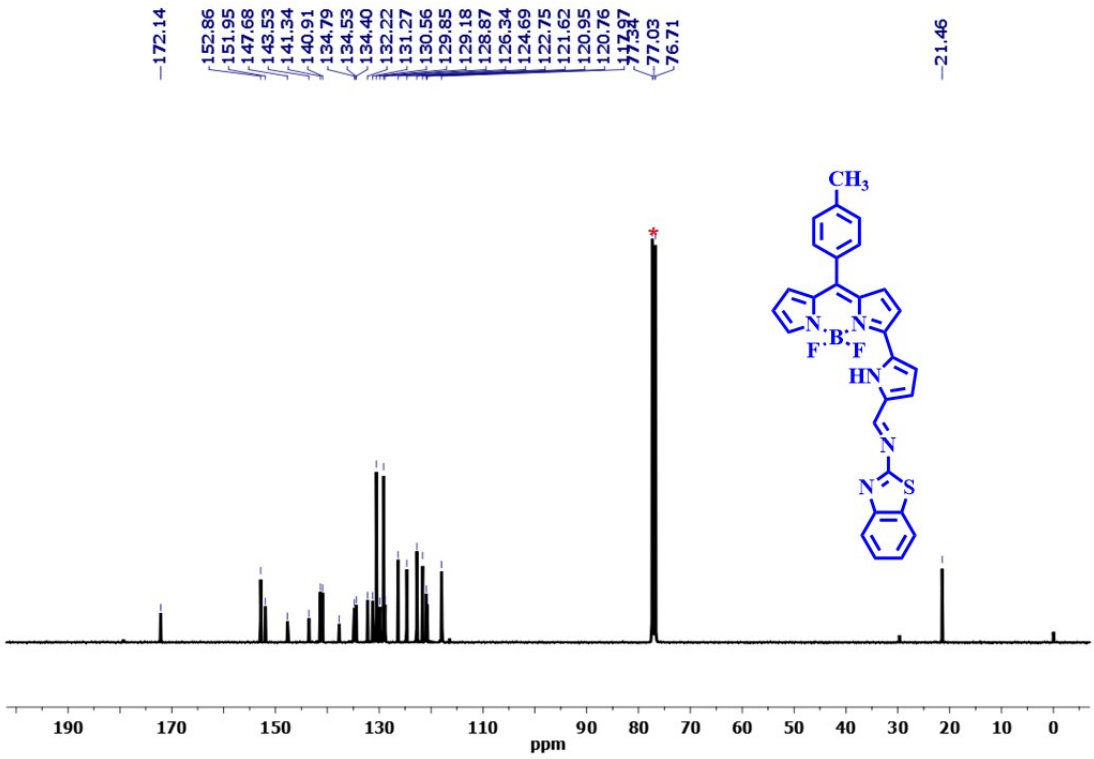


Figure S15. ^{13}C NMR spectrum of the compound **5** recorded in $CDCl_3$. Note: Peaks marked with asterisk (*) are due to residual solvents.

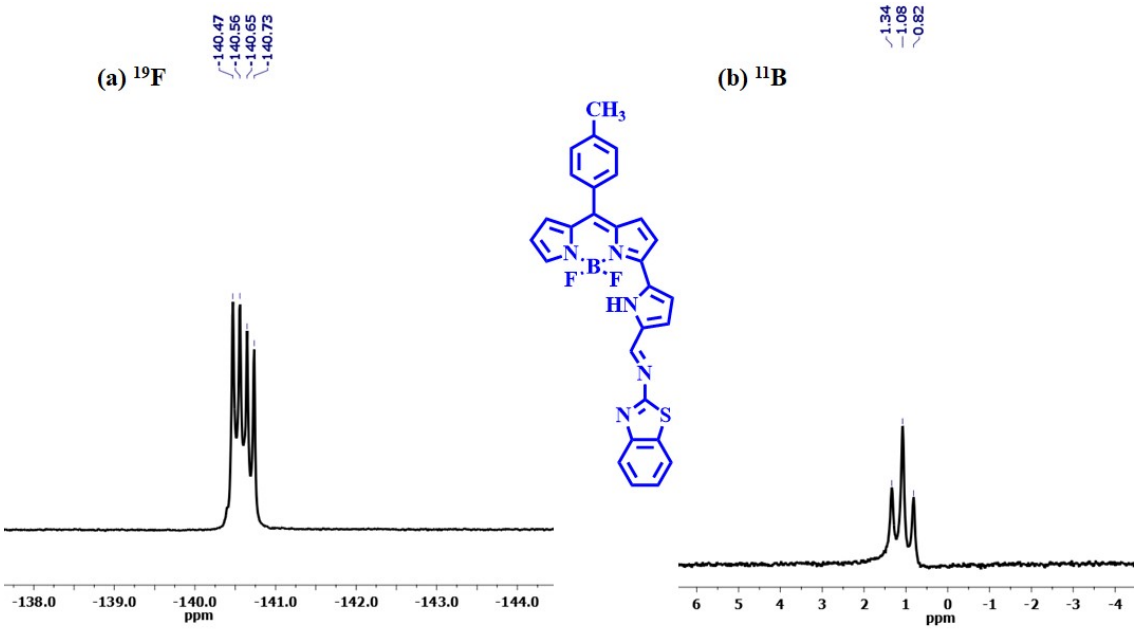


Figure S16. (a) ^{19}F and (b) ^{11}B NMR spectra of the compound **5** recorded in $CDCl_3$.

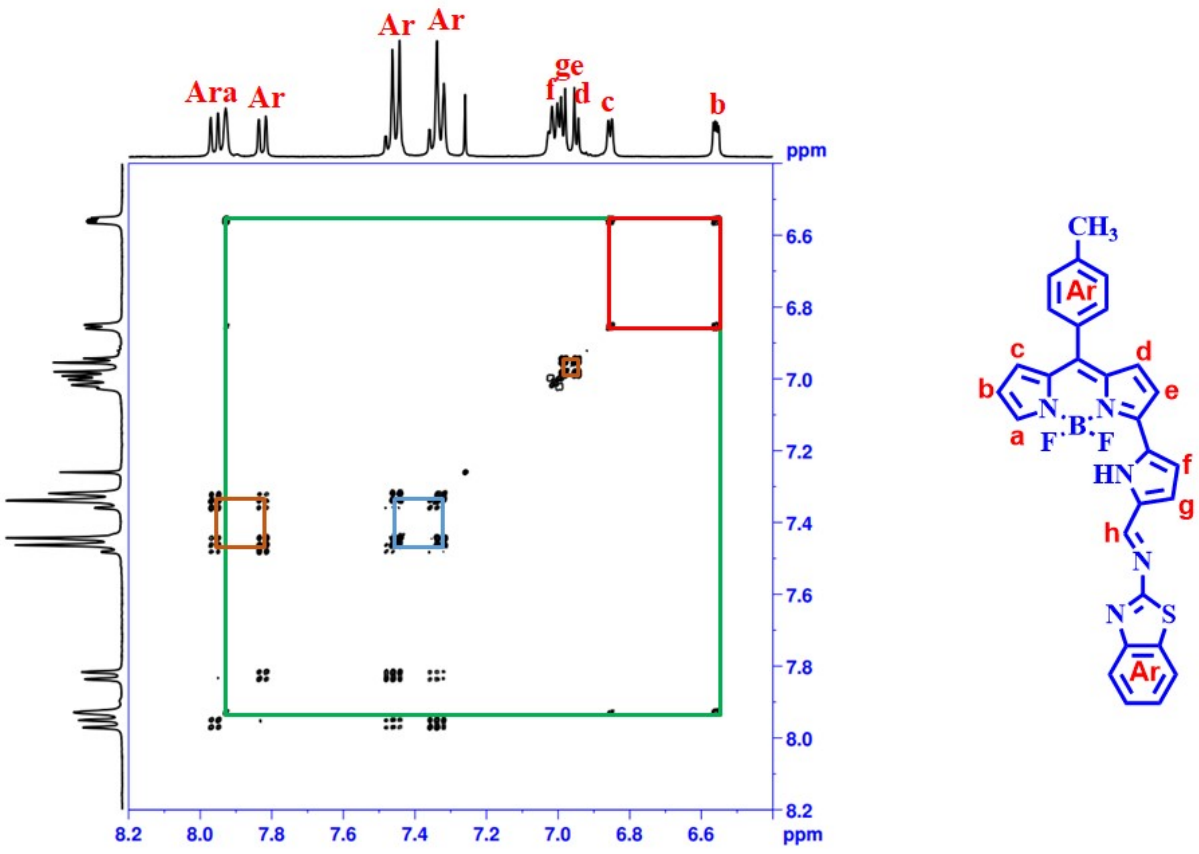


Figure S17. Partial ^{1}H-^{1}H COSY spectrum of the compound **5** in $CDCl_3$ at 25 ˚C.

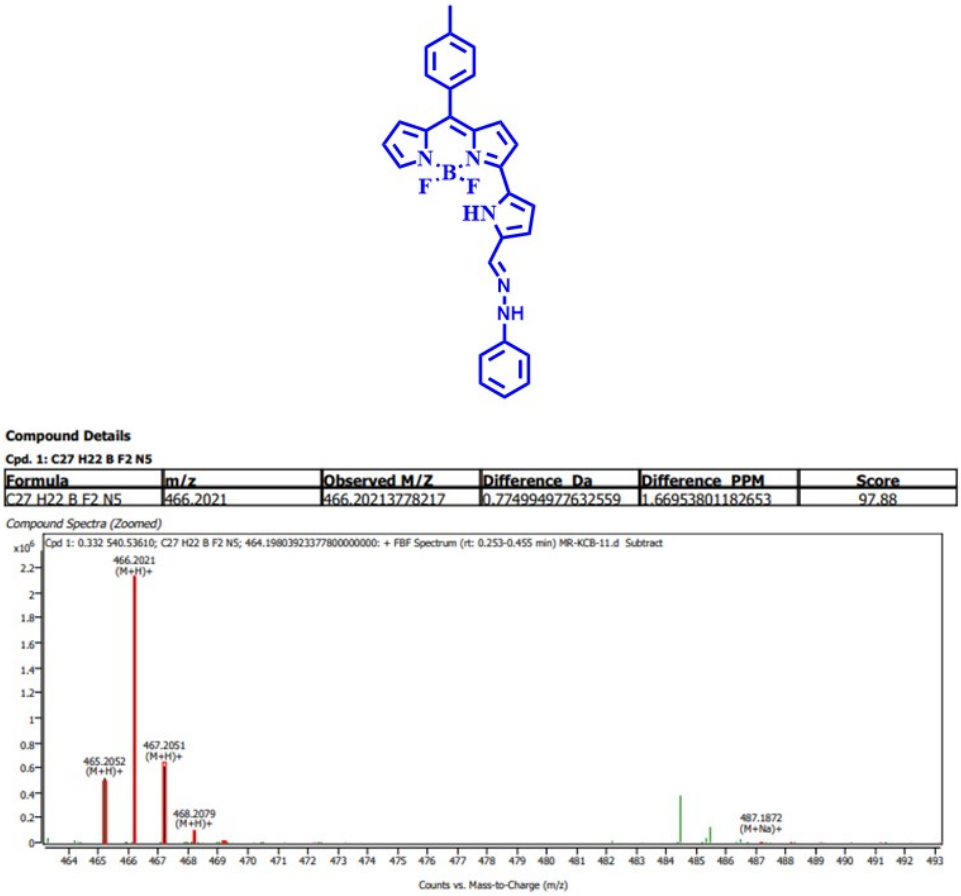


Figure S18. HR mass spectrum of the compound **6**.

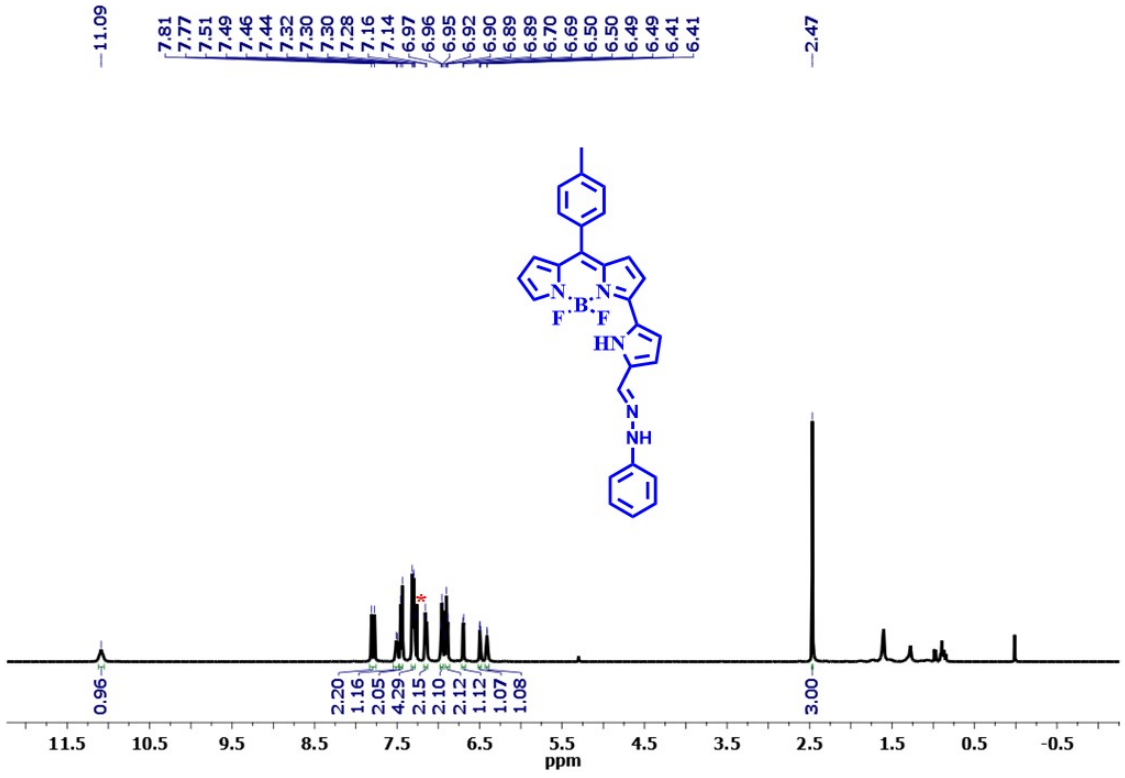


Figure S19. ^{1}H NMR spectrum of the compound **6** recorded in $CDCl_3$ at 25 °C.

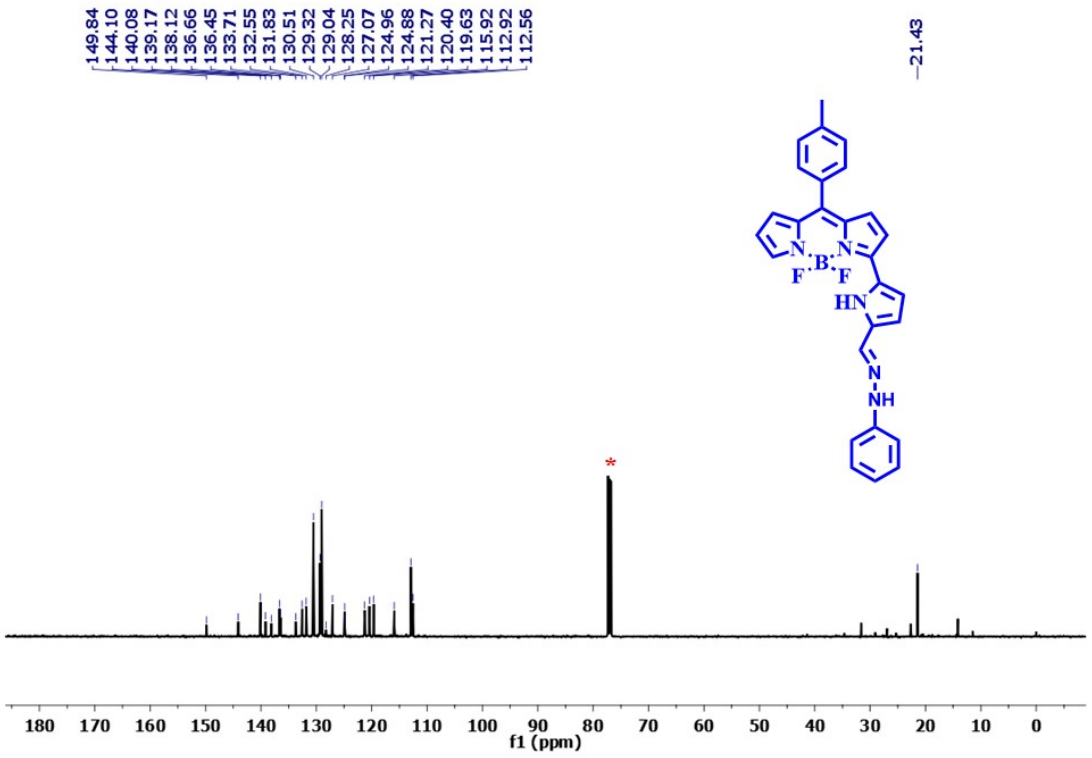


Figure S20. ^{13}C NMR spectrum of the compound **6** recorded in $CDCl_3$. Note: Peaks marked with asterisk (*) are due to residual solvents.

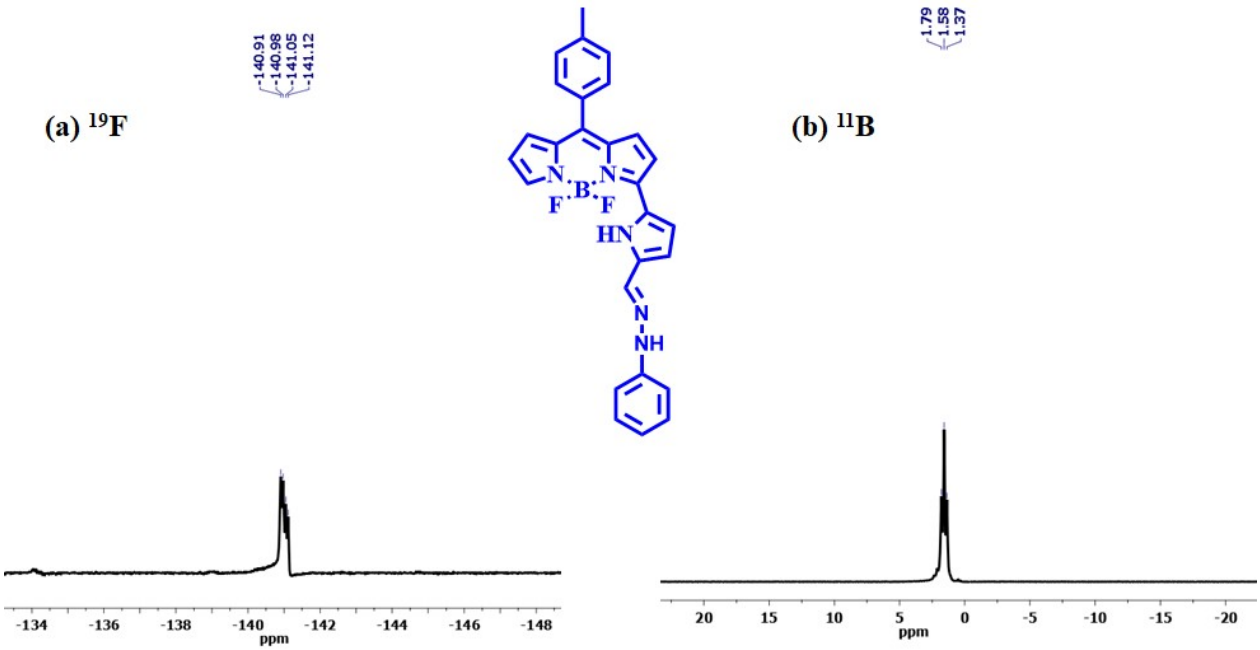


Figure S21. (a) ^{19}F and (b) ^{11}B NMR spectra of the compound **6** recorded in $CDCl_3$.

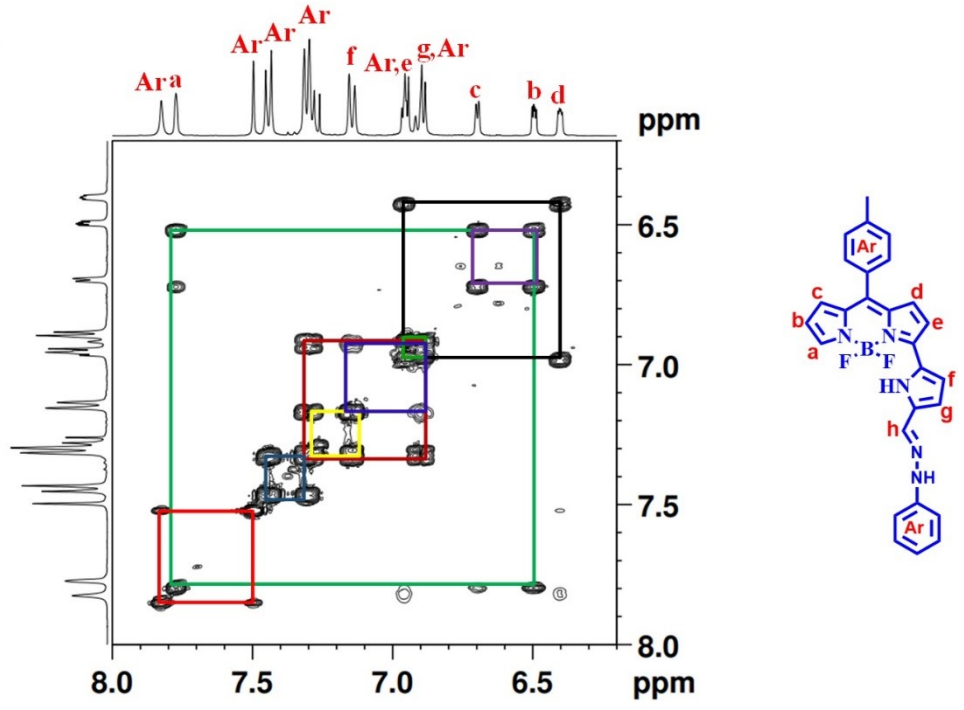


Figure S22. Partial ^{1}H-^{1}H COSY spectrum of the compound **6** in $CDCl_3$ at 25 ˚C.

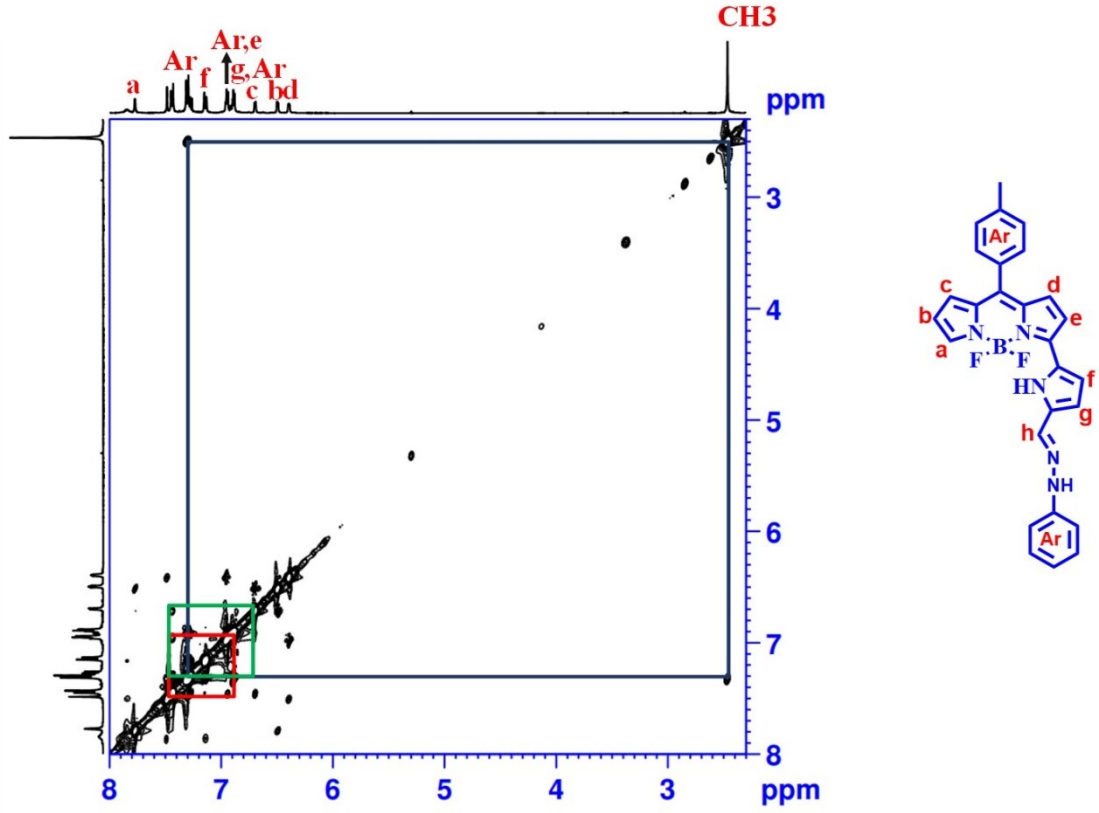
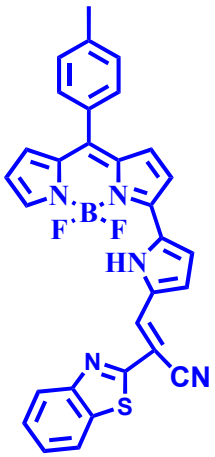


Figure S23. Partial ^{1}H-^{1}H NOESY spectrum of the compound **6** in $CDCl_3$ at 25 ˚C.



Compound Details

Cpd. 1: C30 H20 B F2 N5 S

Formula	m/z	Observed M/Z	Difference_Da	Difference_PPM	Score
C30 H20 B F2 N5 S	532.1576	532.157645147949	-0.31582779593009	-0.595728757382276	98.27

Compound Spectra (Zoomed)

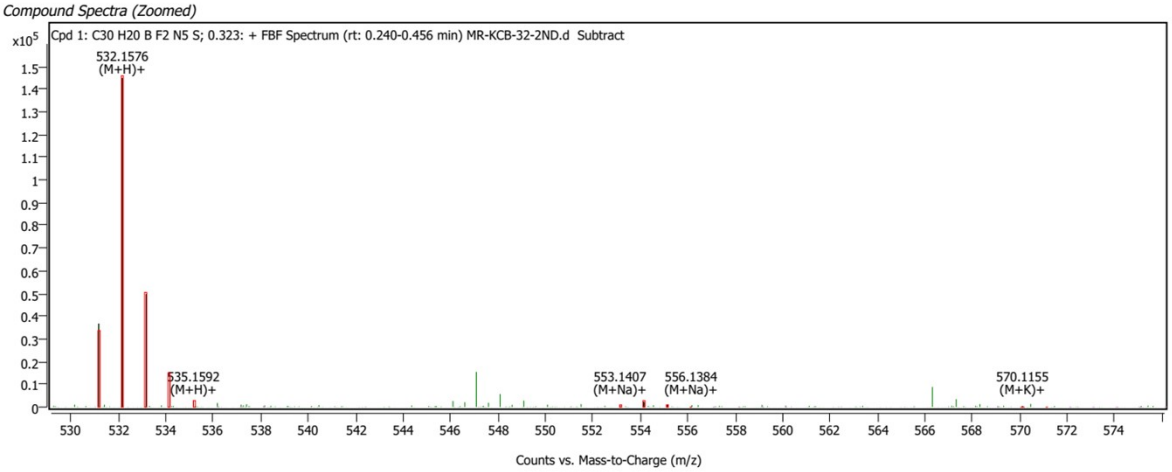


Figure S24. HR mass spectrum of the compound **7**.

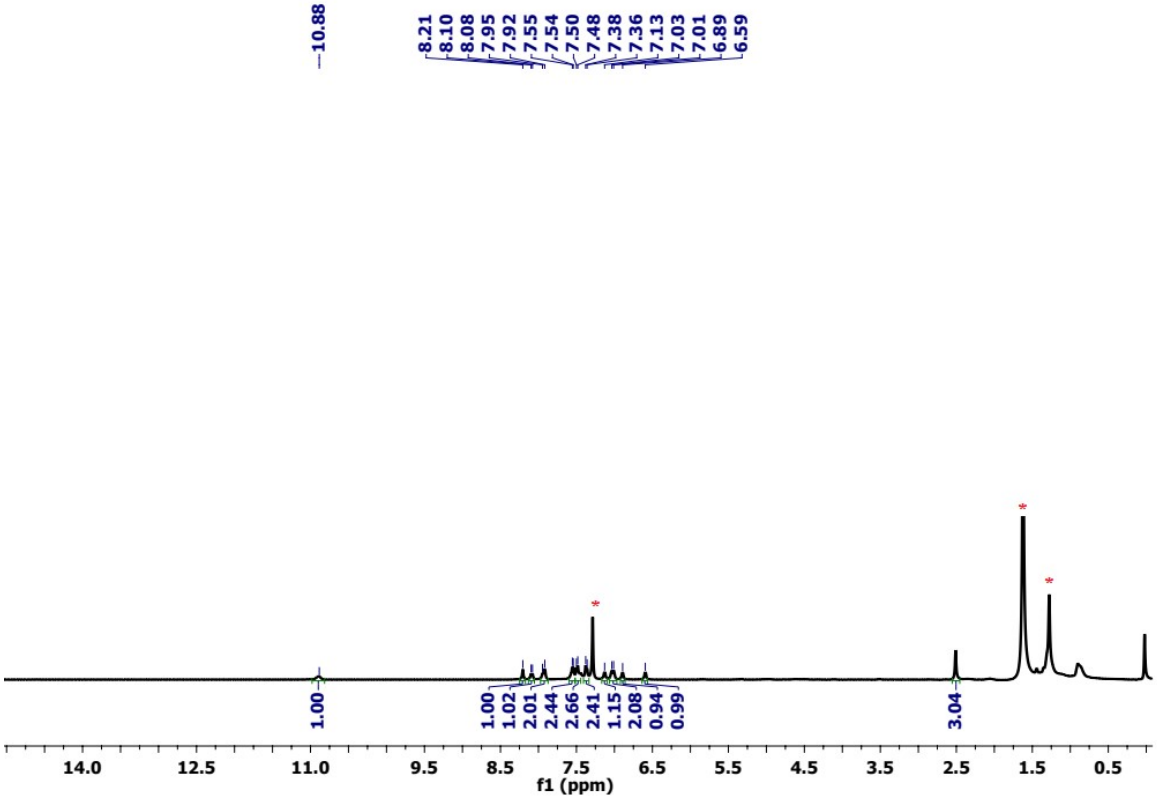


Figure S25. ^{1}H NMR spectrum of the compound **7** recorded in $CDCl_3$ at 25 °C;

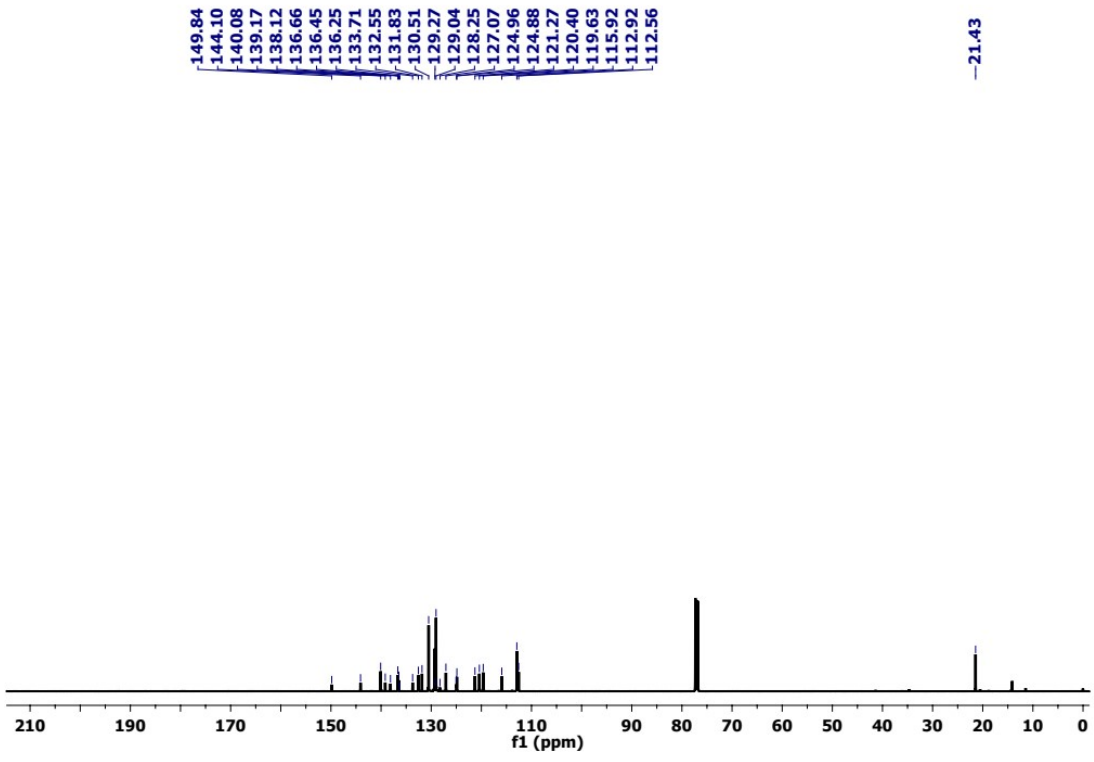
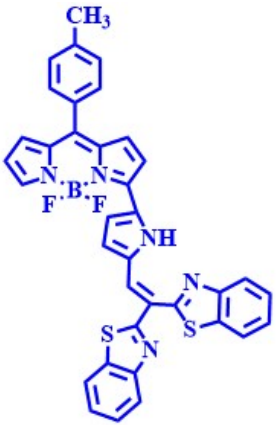


Figure S26. ^{13}C NMR spectrum of the compound **7** recorded in $CDCl_3$ at 25 °C;



Compound Details

Cpd. 1: C36 H24 B F2 N5 S2

Formula	m/z	Observed M/Z	Difference_Da	Difference_PPM	Score
C36 H24 B F2 N5 S2	640.1620	640.161995403131	0.644850122057505	1.01048811767333	98.40

Compound Spectra (Zoomed)

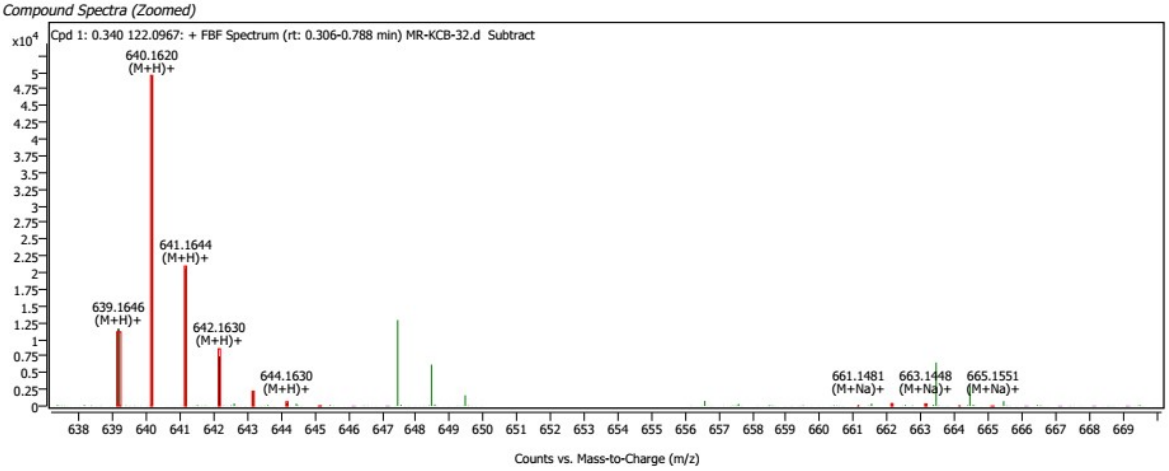


Figure S27. HR mass spectrum of the compound **8**.

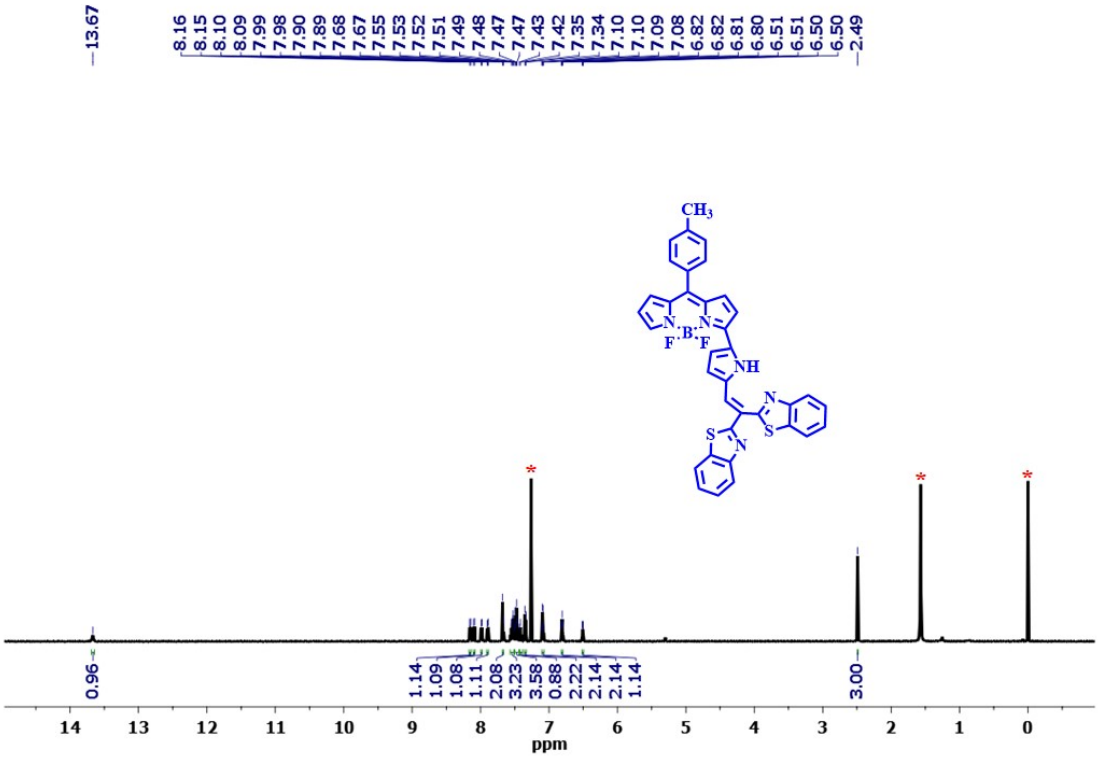


Figure S28. ^{1}H NMR spectrum of the compound **8** recorded in $CDCl_3$ at 25 °C; Note: Peaks marked with asterisk (*) are due to residual solvents.

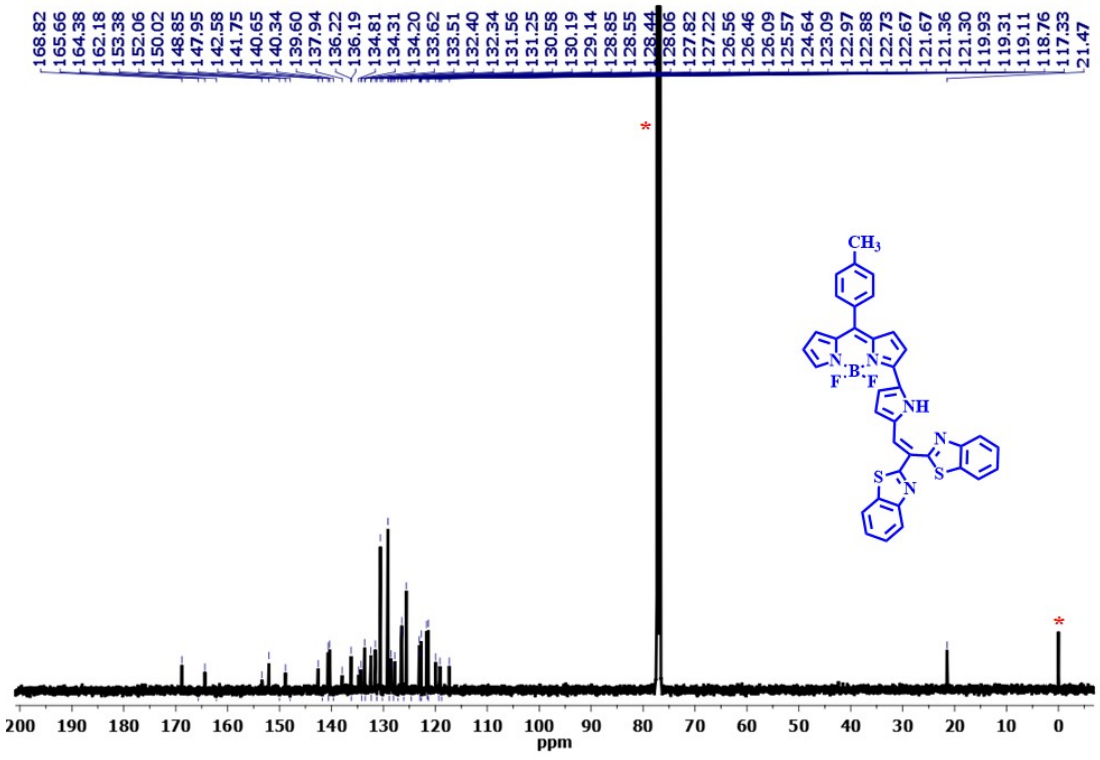


Figure S29. ^{13}C NMR spectrum of the compound **8** recorded in $CDCl_3$. Note: Peaks marked with asterisk (*) are due to residual solvents.

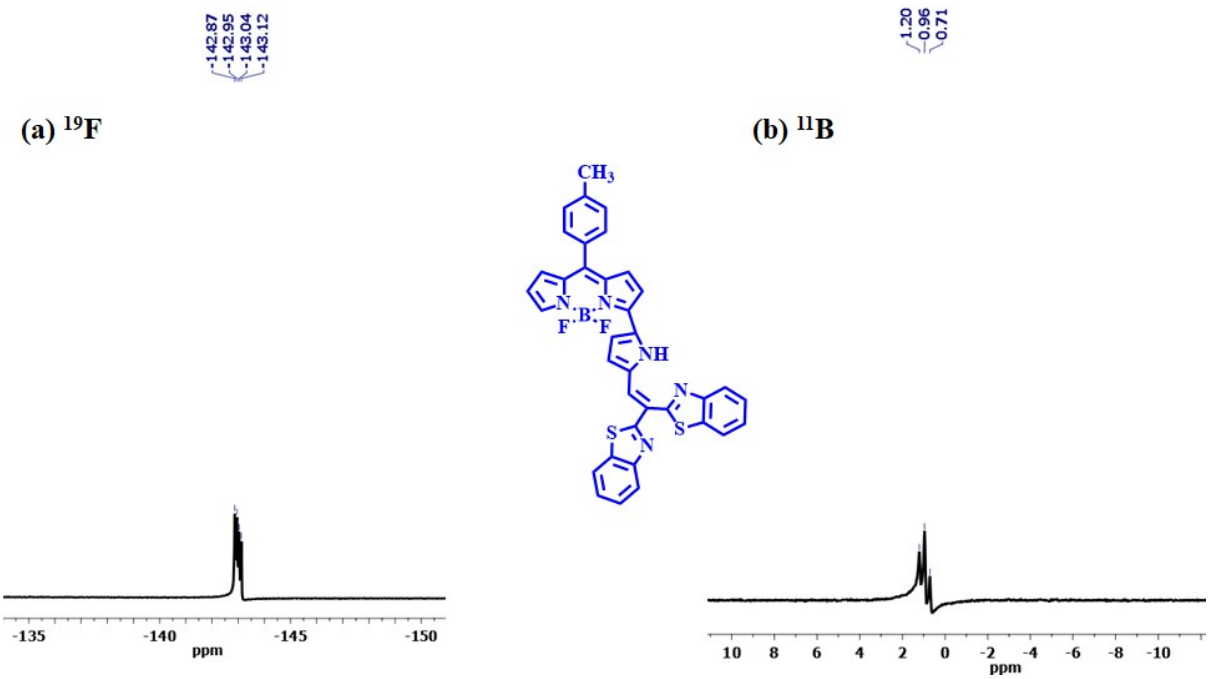


Figure S30. (a) ^{19}F and (b) ^{11}B NMR spectra of the compound **8** recorded in $CDCl_3$.

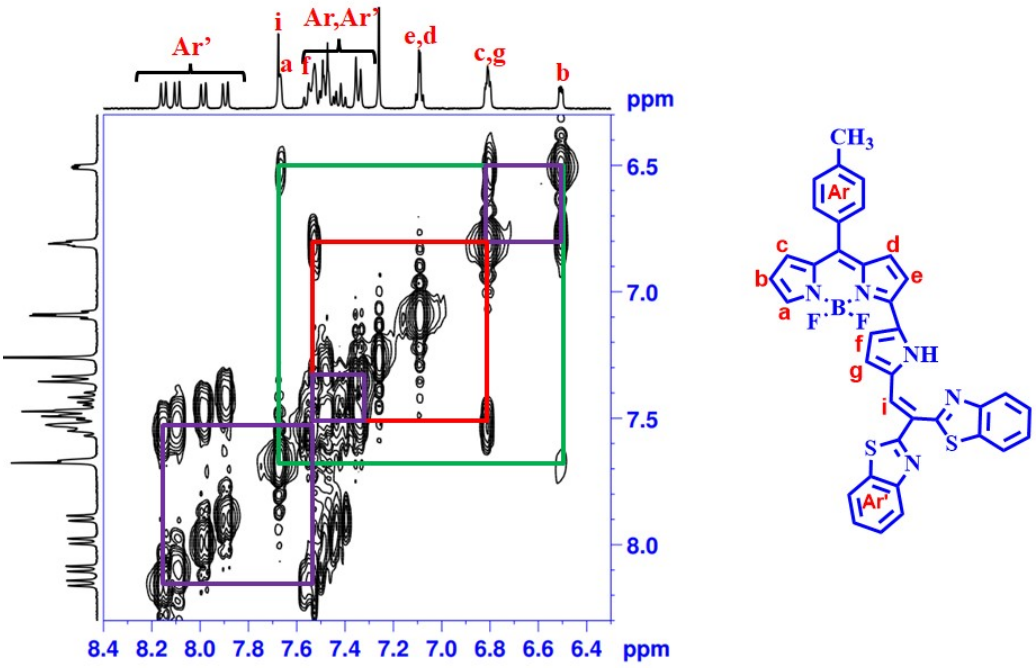


Figure S31. Partial ^{1}H-^{1}H COSY spectrum of the compound **8** in $CDCl_3$ at 25 ˚C.

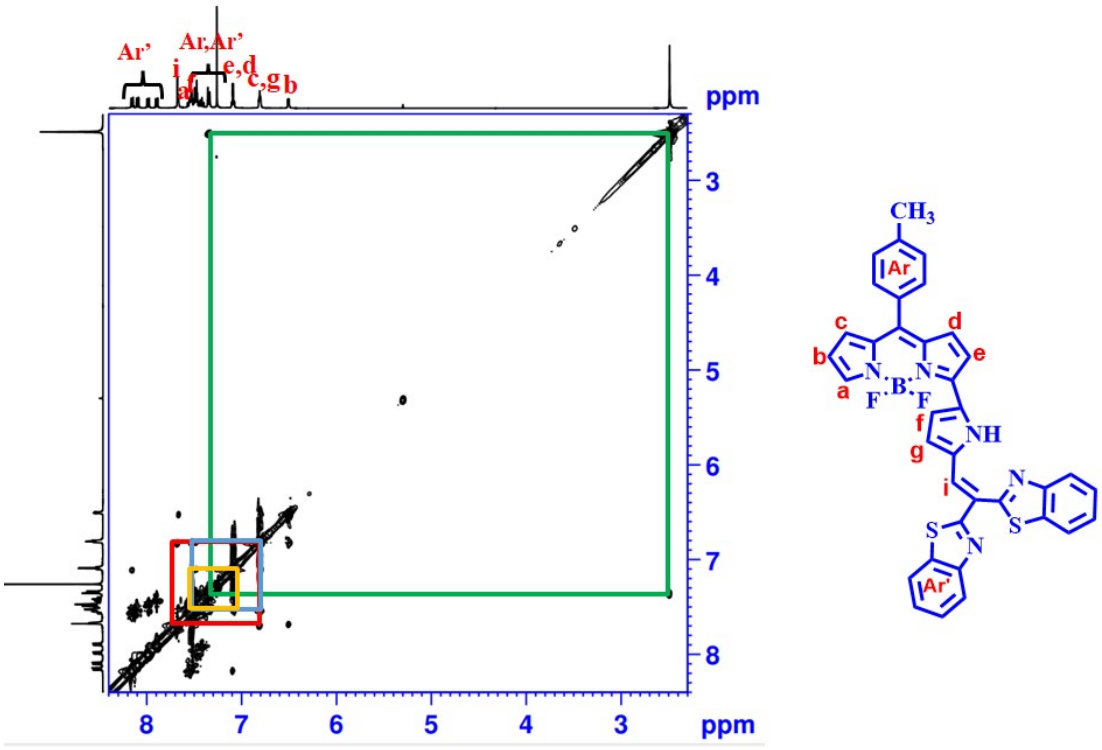


Figure S32. Partial ^{1}H-^{1}H NOESY spectrum of the compound **8** in $CDCl_3$ at 25 ˚C.

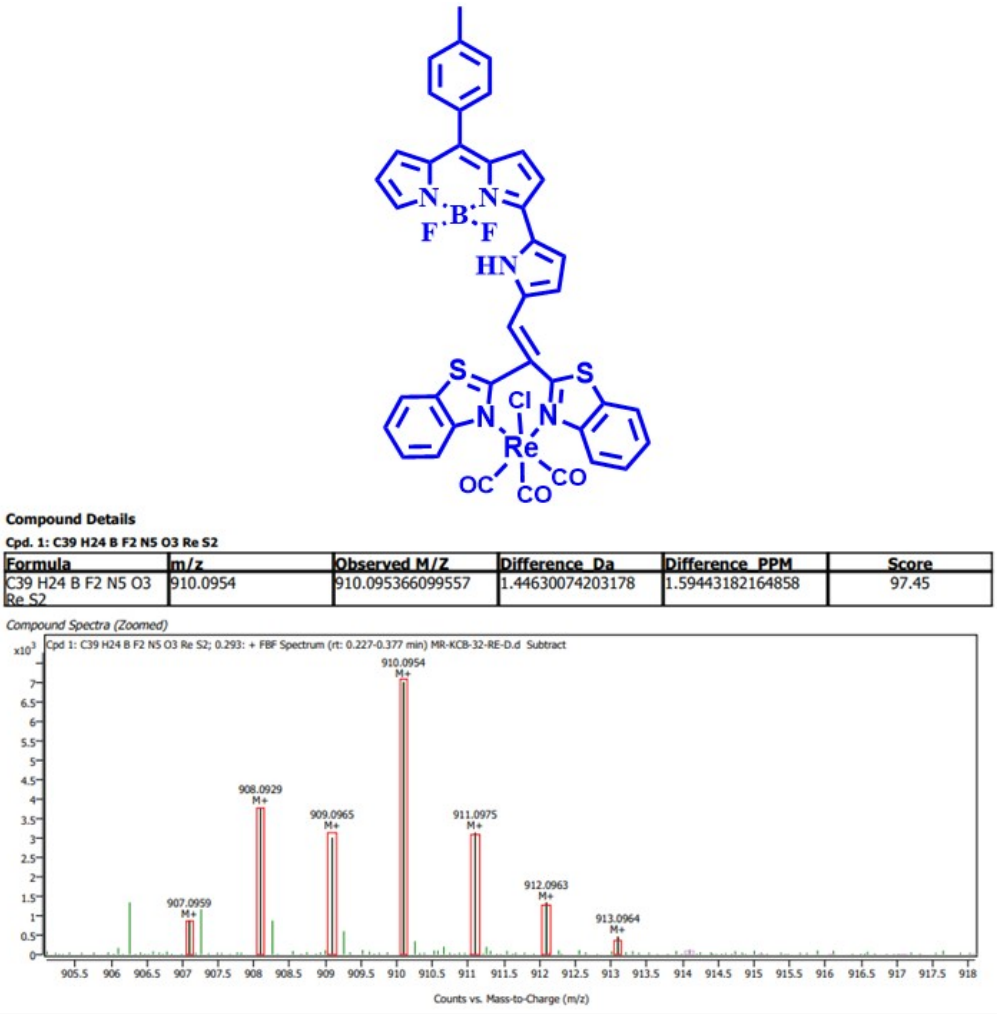


Figure S33. HR mass spectrum of the compound **8-Re(I)**.

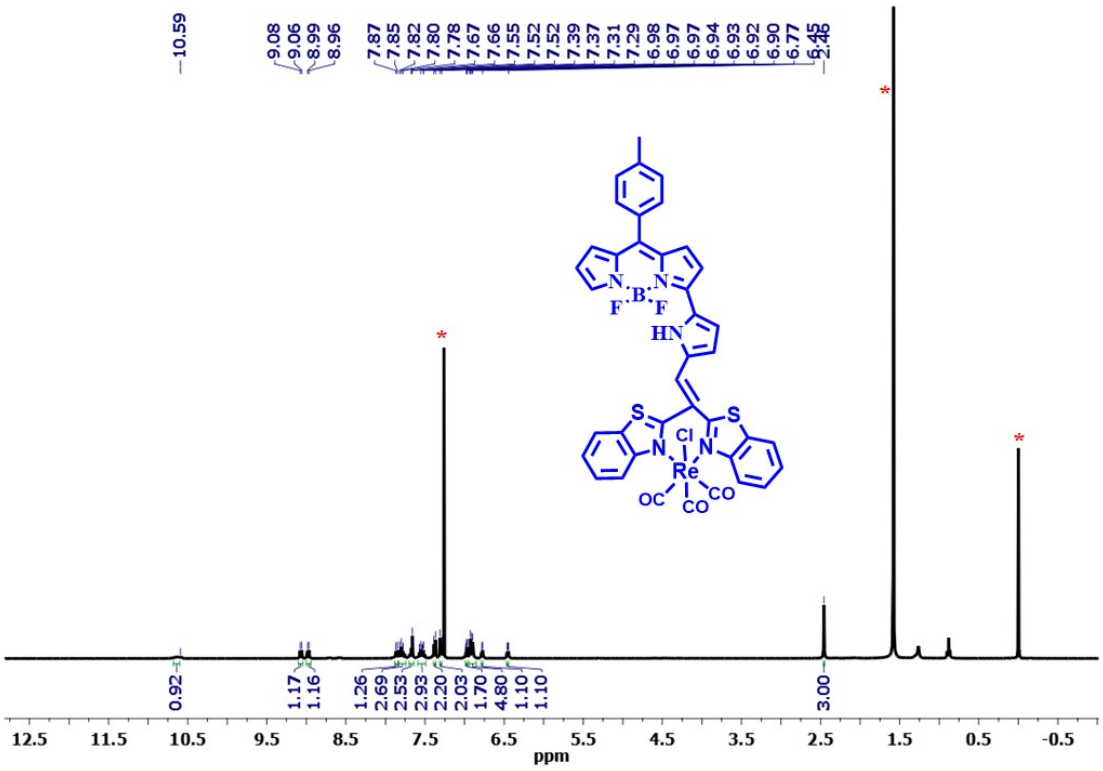


Figure S34. ^{1}H NMR spectrum of the compound **8-Re(I)** recorded in $CDCl_3$ at 25 °C; Note: Peaks marked with asterisk (*) are due to residual solvents.

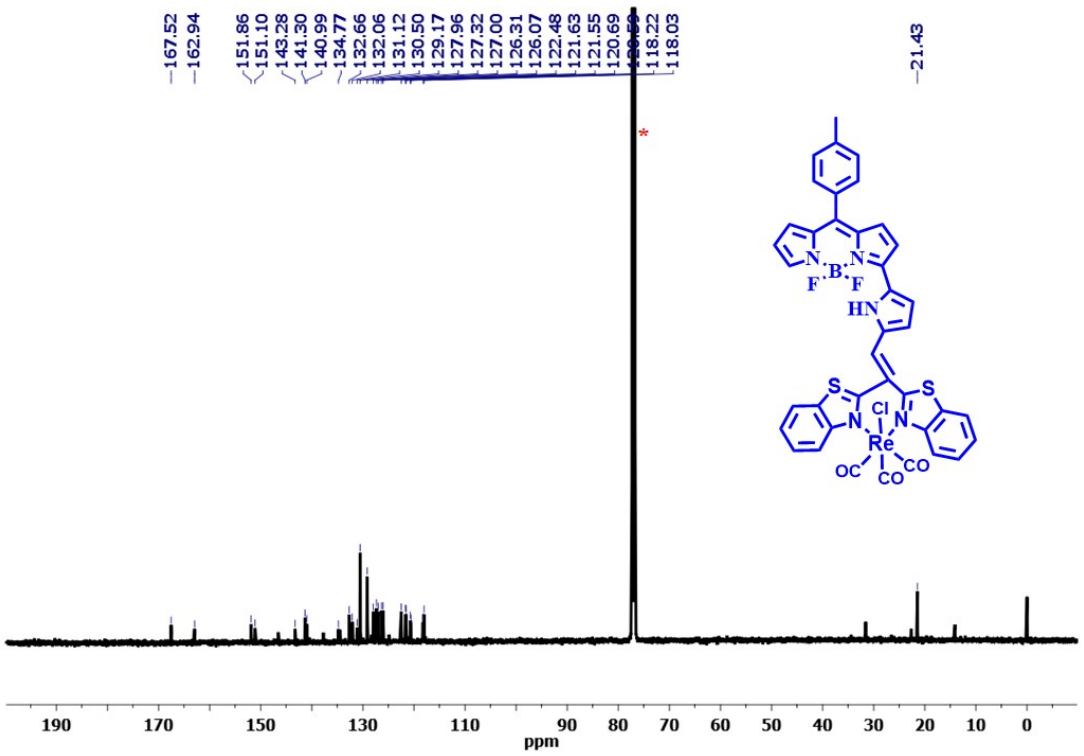


Figure S35. ^{13}C NMR spectrum of the compound **8-Re(I)** recorded in $CDCl_3$. Note: Peaks marked with asterisk (*) are due to residual solvents.

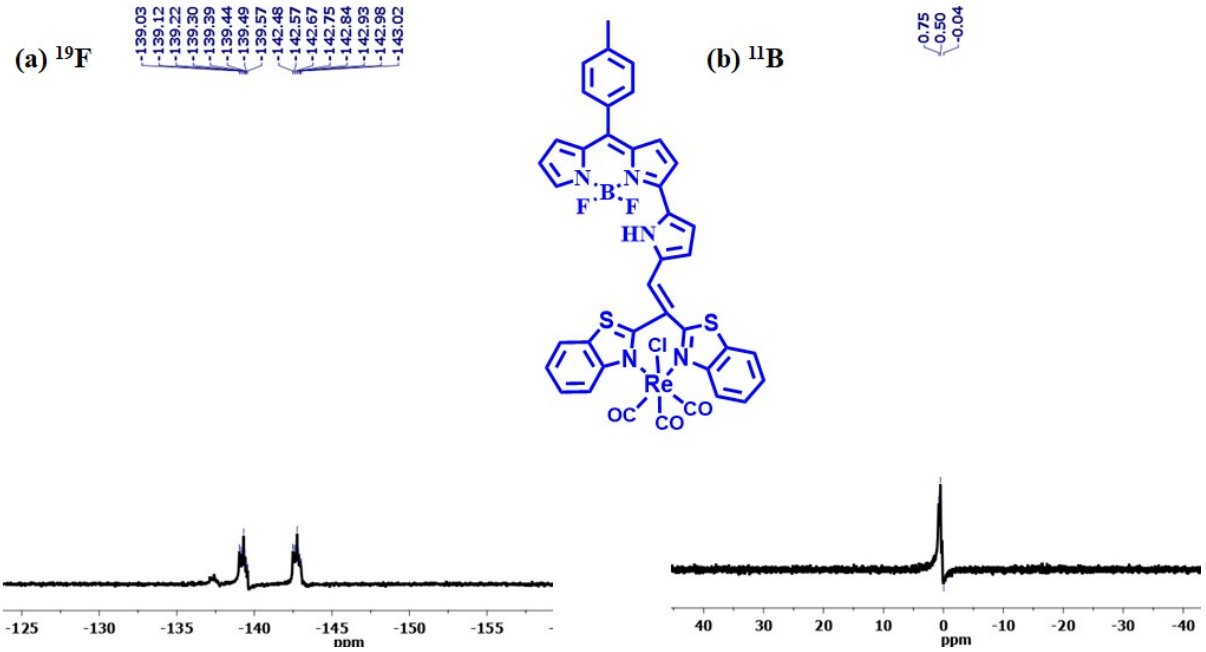


Figure S36. (a) ^{19}F and (b) ^{11}B NMR spectra of the compound **8-Re(I)** recorded in $CDCl_3$.

Table S1. Crystal data and structure refinement for compounds **3**, **6** and **8**.

Parameters	**3**	**8**	**8-Re(I)**
Empirical formula	**$C_{23}H_{18}BF_2N_7$**	**$C_{36}H_{24}BF_2N_5S_2$**	**$C_{39}H_{24}BClF_2N_5O_3ReS_2$**
Formula weight	**441.267**	**640.1620**	**910.09**
Temperature/K	**151(3)**	**150.00(10)**	**150.00(10)**
Crystal system	**Monoclinic**	**monoclinic**	**triclinic**
Space group	**P21/n**	**P21/c**	**P-1**
a/Å	**11.6585(4)**	**22.4102(6)**	**10.6474(3)**
b/Å	**10.0220(3)**	**8.0136(2)**	**13.6874(6)**
c/Å	**18.3087(5)**	**19.3890(4)**	**18.0722(7)**
α/°	**90**	**90**	**74.614(4)**
β/°	**103.006(3)**	**98.932(2)**	**83.007(3)**
γ/°	**90**	**90**	**73.867(3)**
Volume/Å3	**2084.34(11)**	**3439.77(15)**	**2436.08(17)**
Z	**4**	**16**	**2**
ρcalc [g/cm³]	**1.406**	**1.465**	**1.732**
μ/mm⁻¹	**0.100**	**0.436**	**3.020**
F(000)	**912.6**	**1552.0**	**1260.0**
Crystal size/mm³	**0.1 × 0.01 × 0.001**	**0.3 × 0.2 × 0.1**	**0.3 × 0.2 × 0.1**
Radiation	**Mo Kα (λ = 0.71073)**	**Mo Kα (λ =0.71073)**	**Mo Kα (λ = 0.71073)**
2Θ range for data collection/°	**3.8 to 50**	**4.254 to 50**	**3.194 to 50**
Index ranges	**-16 ≤ h ≤ 15, -14 ≤ k ≤ 13, -25 ≤ l ≤ 26**	**-26 ≤ h ≤ 26, -9 ≤ k ≤ 9, -23 ≤ l ≤ 23**	**-12 ≤ h ≤ 12, -16 ≤ k ≤ 16, -21 ≤ l ≤ 21**
Reflections collected	**37818**	**51295**	**66595**
Independent reflections	**3662 [Rint= 0.0902, Rsigma= 0.0718]**	**6045 [Rint= 0.0647, Rsigma= 0.0308]**	**8552 [Rint= 0.0973, Rsigma= 0.0501]**
Data/restraints/parameters Goodness-of-fit on F²	**3662/0/299** **1.018**	**6045/0/452** **1.034**	**8552/6/560** **1.067**
Final R indexes [I>=2σ (I)]	**R1= 0.0435, wR2 = 0.1305**	**R1= 0.0415, wR2 = 0.0981**	**R1= 0.0383, wR2 = 0.0933**
Final R indexes [all data]	**R1= 0.0575, wR2= 0.1446**	**R1= 0.0485, wR2 = 0.1036**	**R1= 0.0421, wR2 = 0.0970**
Largest diff. peak/hole / e Å⁻³	**0.22/-0.27**	**0.81/-0.87**	**1.86/-1.71**

Table S2. Bond Lengths for 3.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
F001	B00X	1.400(2)	C4	C3	1.402(2)
F002	B00X	1.400(2)	C4	C5	1.416(2)
N1	C1	1.354(2)	C5	C17	1.481(2)
N1	C4	1.387(2)	C6	C5	1.396(2)
N1	B00X	1.520(2)	C6	C7	1.416(2)
N2	C6	1.407(2)	C8	C7	1.365(2)
N2	C9	1.363(2)	C8	C9	1.422(2)
N2	B00X	1.549(2)	C9	C10	1.431(2)
N3	C10	1.367(2)	C10	C11	1.395(2)
N3	C13	1.362(2)	C11	C12	1.394(3)
N4	C14	1.290(2)	C12	C13	1.390(3)
N5	N4	1.389(2)	C14	C13	1.434(2)
N5	C15	1.355(2)	C17	C18	1.405(2)
N5	C16	1.367(2)	C18	C19	1.387(2)
N6	N7	1.399(2)	C20	C19	1.393(3)
N6	C15	1.303(2)	C20	C21	1.387(3)
N7	C16	1.305(2)	C20	C23	1.508(2)
C1	C2	1.384(2)	C22	C17	1.391(3)
C3	C2	1.394(2)	C22	C21	1.387(2)

Table S3. Bond Angles for 3.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C1	N1	C4	107.48(14)	C10	C9	C8	124.09(16)
B00X	N1	C1	125.93(15)	C9	C10	N3	125.76(16)
B00X	N1	C4	126.50(15)	C11	C10	N3	106.49(15)
C6	N2	C9	107.89(14)	C11	C10	C9	127.73(16)
B00X	N2	C6	123.51(14)	C12	C11	C10	108.20(16)
B00X	N2	C9	128.57(14)	C13	C12	C11	107.33(16)
C13	N3	C10	110.55(15)	C12	C13	N3	107.44(15)
C14	N4	N5	117.23(15)	C12	C13	C14	131.48(17)
C15	N5	N4	121.41(15)	C14	C13	N3	121.06(16)
C16	N5	N4	133.33(16)	C13	C14	N4	117.37(16)
C16	N5	C15	105.24(16)	N6	C15	N5	110.86(18)
C15	N6	N7	106.60(16)	N7	C16	N5	109.85(18)
C16	N7	N6	107.44(17)	C18	C17	C5	120.04(16)
C2	C1	N1	110.41(16)	C18	C17	C22	118.05(16)
C3	C2	C1	106.70(16)	C22	C17	C5	121.86(16)
C2	C3	C4	107.33(16)	C19	C18	C17	120.33(17)
C3	C4	N1	108.06(15)	C18	C19	C20	121.52(17)
C3	C4	C5	131.73(17)	C19	C20	C21	117.74(17)
C5	C4	N1	120.20(15)	C23	C20	C19	120.44(17)
C4	C5	C6	119.69(16)	C23	C20	C21	121.82(17)
C17	C5	C4	119.29(15)	C22	C21	C20	121.47(17)
C17	C5	C6	121.01(16)	C21	C22	C17	120.88(17)
C5	C6	N2	122.00(15)	F002	B00X	F001	107.88(15)
C7	C6	N2	107.56(15)	N1	B00X	F001	110.80(15)
C7	C6	C5	130.44(16)	N1	B00X	F002	110.35(15)
C6	C7	C8	107.97(16)	N2	B00X	F001	109.56(15)
C7	C8	C9	107.90(16)	N2	B00X	F002	110.40(15)

C8	C9	N2	108.65(15)	N2	B00X	N1	107.86(14)
C10	C9	N2	127.25(15)				

Table S4. Bond Lengths for 8.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cl03	C01C	1.748(3)	C9	C10	1.439(3)
Cl04	C01C	1.756(3)	C10	C11	1.406(3)
Cl05	C01C	1.732(3)	C11	C12	1.386(3)
S1	C16	1.770(2)	C13	C12	1.406(3)
S1	C22	1.736(2)	C13	C14	1.427(3)
S2	C23	1.770(2)	C15	C14	1.374(3)
S2	C29	1.732(2)	C15	C16	1.473(3)
F1	B1	1.401(3)	C15	C23	1.473(3)
F2	B1	1.378(3)	C17	C18	1.406(3)
N1	C1	1.353(3)	C17	C22	1.400(3)
N1	C4	1.390(3)	C18	C19	1.382(3)
N1	B1	1.550(3)	C19	C20	1.398(3)
N2	C6	1.406(3)	C21	C20	1.389(3)
N2	C9	1.360(3)	C21	C22	1.398(3)
N2	B1	1.566(3)	C24	C25	1.400(3)
N3	C10	1.368(3)	C24	C29	1.404(3)
N3	C13	1.364(3)	C25	C26	1.384(3)
N4	C23	1.298(3)	C26	C27	1.398(4)
N4	C24	1.395(3)	C28	C27	1.384(3)
N5	C16	1.315(3)	C29	C28	1.398(3)
N5	C17	1.385(3)	C30	C5	1.491(3)
C1	C2	1.389(4)	C30	C31	1.393(3)
C3	C2	1.391(4)	C30	C35	1.389(3)
C4	C3	1.405(3)	C31	C32	1.389(4)
C5	C4	1.409(3)	C32	C33	1.376(4)
C6	C5	1.387(3)	C33	C36	1.520(4)
C6	C7	1.420(3)	C34	C33	1.383(4)
C8	C7	1.363(3)	C35	C34	1.394(4)
C8	C9	1.424(3)			

Table S5. Bond Angles for 8.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
Cl03	C01C	Cl04	109.77(14)	N5	C16	S1	113.99(15)
Cl05	C01C	Cl03	110.91(16)	N5	C16	C15	123.26(18)
Cl05	C01C	Cl04	110.90(16)	C15	C16	S1	122.75(15)
C22	S1	C16	89.27(10)	N5	C17	C18	125.18(19)
C29	S2	C23	89.29(10)	N5	C17	C22	114.61(18)
C1	N1	C4	107.6(2)	C22	C17	C18	120.22(19)
C1	N1	B1	125.8(2)	C19	C18	C17	118.2(2)
C4	N1	B1	126.56(19)	C18	C19	C20	121.3(2)
C6	N2	B1	123.14(18)	C21	C20	C19	121.1(2)
C9	N2	C6	107.17(17)	C20	C21	C22	117.8(2)
C9	N2	B1	129.56(18)	C17	C22	S1	110.04(15)
C13	N3	C10	110.29(17)	C21	C22	S1	128.65(17)
C23	N4	C24	111.48(17)	C21	C22	C17	121.30(19)

C16	N5	C17	112.06(17)	N4	C23	S2	114.79(15)
N1	C1	C2	110.0(2)	N4	C23	C15	124.21(18)
C1	C2	C3	107.1(2)	C15	C23	S2	121.00(15)
C2	C3	C4	107.2(2)	N4	C24	C25	125.6(2)
N1	C4	C3	108.1(2)	N4	C24	C29	114.80(19)
N1	C4	C5	120.1(2)	C25	C24	C29	119.6(2)
C3	C4	C5	131.7(2)	C26	C25	C24	118.7(2)
C4	C5	C30	121.3(2)	C25	C26	C27	121.0(2)
C6	C5	C4	120.2(2)	C28	C27	C26	121.3(2)
C6	C5	C30	118.5(2)	C27	C28	C29	117.6(2)
N2	C6	C7	108.20(18)	C24	C29	S2	109.62(15)
C5	C6	N2	122.8(2)	C28	C29	S2	128.70(18)
C5	C6	C7	129.0(2)	C28	C29	C24	121.7(2)
C8	C7	C6	107.55(19)	C31	C30	C5	119.6(2)
C7	C8	C9	107.79(19)	C35	C30	C5	121.9(2)
N2	C9	C8	109.28(18)	C35	C30	C31	118.3(2)
N2	C9	C10	126.55(19)	C32	C31	C30	120.6(3)
C8	C9	C10	124.16(19)	C33	C32	C31	121.2(3)
N3	C10	C9	118.79(18)	C32	C33	C34	118.4(2)
N3	C10	C11	107.49(18)	C32	C33	C36	120.5(3)
C11	C10	C9	133.7(2)	C34	C33	C36	121.1(3)
C12	C11	C10	107.01(19)	C33	C34	C35	121.2(3)
C11	C12	C13	108.44(19)	C30	C35	C34	120.3(3)
N3	C13	C12	106.75(18)	F1	B1	N1	109.64(19)
N3	C13	C14	128.13(19)	F1	B1	N2	109.70(19)
C12	C13	C14	125.12(19)	F2	B1	F1	110.06(19)
C15	C14	C13	137.05(19)	F2	B1	N1	109.7(2)
C14	C15	C16	125.42(18)	F2	B1	N2	111.03(19)
C14	C15	C23	116.80(18)	N1	B1	N2	106.67(18)
C16	C15	C23	117.76(18)				

Table S6 Bond Lengths for 8-Re(I) complex.

Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
Re1	Cl1	2.4998(14)	C9	C10	1.440(7)
Re1	N4	2.205(4)	C10	C11	1.401(7)
Re1	N5	2.222(4)	C12	C11	1.396(7)
Re1	C37	1.935(5)	C13	C12	1.400(7)
Re1	C38	1.977(5)	C13	C14	1.424(7)
Re1	C39	1.912(5)	C15	C14	1.354(7)
S1	C16	1.734(4)	C15	C16	1.469(6)
S1	C22	1.735(5)	C17	C18	1.391(7)
S2	C23	1.734(4)	C17	C22	1.413(6)
S2	C29	1.735(5)	C18	C19	1.393(6)
F1	B1	1.389(7)	C19	C20	1.402(7)
F2	B1	1.394(7)	C21	C20	1.375(7)
O1	C39	1.163(6)	C22	C21	1.395(6)
O2	C38	1.012(6)	C23	C15	1.480(6)
O3	C37	1.145(6)	C25	C24	1.404(7)
N1	C1	1.339(6)	C25	C26	1.371(7)

N1	C4	1.393(6)	C27	C26	1.402(7)
N1	B1	1.544(7)	C27	C28	1.385(7)
N2	C6	1.404(6)	C29	C24	1.397(7)
N2	C9	1.365(6)	C29	C28	1.398(6)
N2	B1	1.562(7)	C30	C5	1.489(7)
N3	C10	1.359(6)	C30	C31	1.392(7)
N3	C13	1.374(6)	C31	C32	1.398(8)
N4	C23	1.317(6)	C33	C32	1.389(8)
N4	C24	1.404(6)	C33	C36	1.508(7)
N5	C16	1.321(6)	C34	C33	1.385(8)
N5	C17	1.407(6)	C35	C30	1.396(7)
C1	C2	1.405(7)	C35	C34	1.395(7)
C3	C2	1.386(7)	Cl00	C01N	1.755(6)
C4	C3	1.409(7)	Cl4	C01N	1.763(6)
C5	C4	1.405(7)	Cl5	C01N	1.749(5)
C5	C6	1.387(7)	Cl2	C01S	1.752(6)
C6	C7	1.422(7)	Cl3	C01S	1.755(7)
C8	C7	1.358(7)	Cl6	C01S	1.750(7)
C9	C8	1.417(7)			

Table S7. Bond Angles for 8-Re(I) complex

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N4	Re1	Cl1	87.41(10)	C15	C14	C13	130.4(4)
N4	Re1	N5	81.98(13)	C14	C15	C16	119.7(4)
N5	Re1	Cl1	86.88(10)	C14	C15	C23	124.4(4)
C37	Re1	Cl1	94.69(15)	C16	C15	C23	115.8(4)
C37	Re1	N4	174.61(16)	N5	C16	S1	115.8(3)
C37	Re1	N5	93.16(16)	N5	C16	C15	123.8(4)
C37	Re1	C38	89.72(19)	C15	C16	S1	120.3(3)
C38	Re1	Cl1	175.50(13)	N5	C17	C22	113.4(4)
C38	Re1	N4	88.27(16)	C18	C17	N5	127.3(4)
C38	Re1	N5	93.74(17)	C18	C17	C22	119.3(4)
C39	Re1	Cl1	91.92(15)	C17	C18	C19	119.2(4)
C39	Re1	N4	97.09(16)	C18	C19	C20	120.4(5)
C39	Re1	N5	178.51(16)	C21	C20	C19	121.5(4)
C39	Re1	C37	87.81(19)	C20	C21	C22	118.0(4)
C39	Re1	C38	87.4(2)	C17	C22	S1	110.4(3)
C16	S1	C22	89.4(2)	C21	C22	S1	128.0(4)
C23	S2	C29	89.5(2)	C21	C22	C17	121.6(4)
C1	N1	C4	107.7(4)	N4	C23	S2	115.1(3)
C1	N1	B1	125.4(4)	N4	C23	C15	125.8(4)
C4	N1	B1	126.8(4)	C15	C23	S2	118.9(3)
C6	N2	B1	122.5(4)	N4	C24	C25	126.6(4)
C9	N2	C6	107.2(4)	C29	C24	N4	113.7(4)
C9	N2	B1	129.7(4)	C29	C24	C25	119.6(4)
C10	N3	C13	110.9(4)	C26	C25	C24	118.0(4)
C23	N4	Re1	120.2(3)	C25	C26	C27	122.1(5)
C23	N4	C24	111.2(4)	C28	C27	C26	120.9(4)
C24	N4	Re1	128.5(3)	C27	C28	C29	116.9(4)

C16	N5	Re1	120.8(3)	C24	C29	S2	110.2(3)
C16	N5	C17	110.9(4)	C24	C29	C28	122.5(4)
C17	N5	Re1	127.0(3)	C28	C29	S2	127.2(4)
N1	C1	C2	110.7(4)	C31	C30	C5	121.4(5)
C3	C2	C1	106.0(5)	C31	C30	C35	118.8(5)
C2	C3	C4	107.9(4)	C35	C30	C5	119.8(5)
N1	C4	C3	107.7(4)	C30	C31	C32	120.2(5)
N1	C4	C5	119.5(4)	C33	C32	C31	121.0(6)
C5	C4	C3	132.7(5)	C32	C33	C36	120.8(6)
C4	C5	C30	119.9(4)	C34	C33	C32	118.7(5)
C6	C5	C4	120.4(4)	C34	C33	C36	120.5(6)
C6	C5	C30	119.5(4)	C33	C34	C35	120.8(5)
N2	C6	C7	108.0(4)	C34	C35	C30	120.5(5)
C5	C6	N2	123.0(5)	O3	C37	Re1	177.5(4)
C5	C6	C7	129.0(4)	O2	C38	Re1	177.1(4)
C8	C7	C6	107.7(4)	O1	C39	Re1	177.8(4)
C7	C8	C9	108.0(5)	F1	B1	F2	109.3(4)
N2	C9	C8	109.2(4)	F1	B1	N1	109.5(5)
N2	C9	C10	126.3(5)	F1	B1	N2	112.4(5)
C8	C9	C10	124.4(5)	F2	B1	N1	110.5(5)
N3	C10	C9	125.6(4)	F2	B1	N2	108.1(4)
N3	C10	C11	107.2(4)	N1	B1	N2	107.1(4)
C11	C10	C9	127.0(5)	Cl00	C01N	Cl4	111.1(3)
C12	C11	C10	107.4(5)				
C11	C12	C13	108.1(4)				
N3	C13	C12	106.4(4)				
N3	C13	C14	125.0(4)				
C12	C13	C14	128.5(4)				

Table S8. Selected bond angles in the crystal structures of **3**, **8** and **8-Re(I)**.

	Various bond angles of 3, 8 and 8-Re(I)				
Comp.	<N2-B1-N2	<F2-B1-F1	<F1-B1-N2	<F2-B1-N2	<F2-B1-N1
3	⊃ 107.87°	⊃107.85°	⊃ 110.42°	⊃109.57°	⊃ 110.79°
8	⊃ 106.66°	⊃ 110.07°	⊃ 109.70°	⊃ 109.70°	⊃ 109.67°
8-Re(I)	⊃ 107.19°	⊃ 109.26°	⊃ 108.08°	⊃ 112.48°	⊃ 109.45°

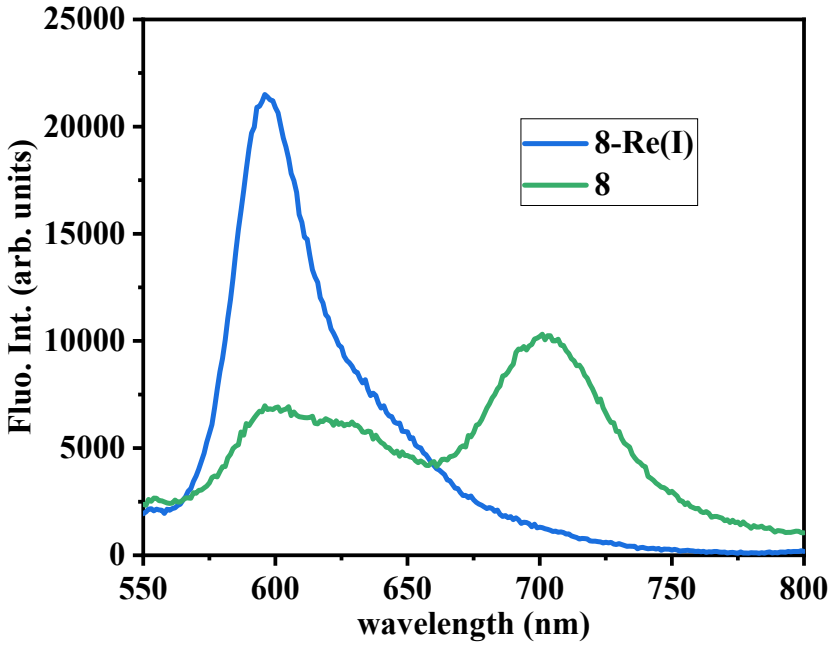


Fig. S37. Emission spectra of compounds **8** and **8-Re(I)** upon excitation at 530 nm in CH_2Cl_2.

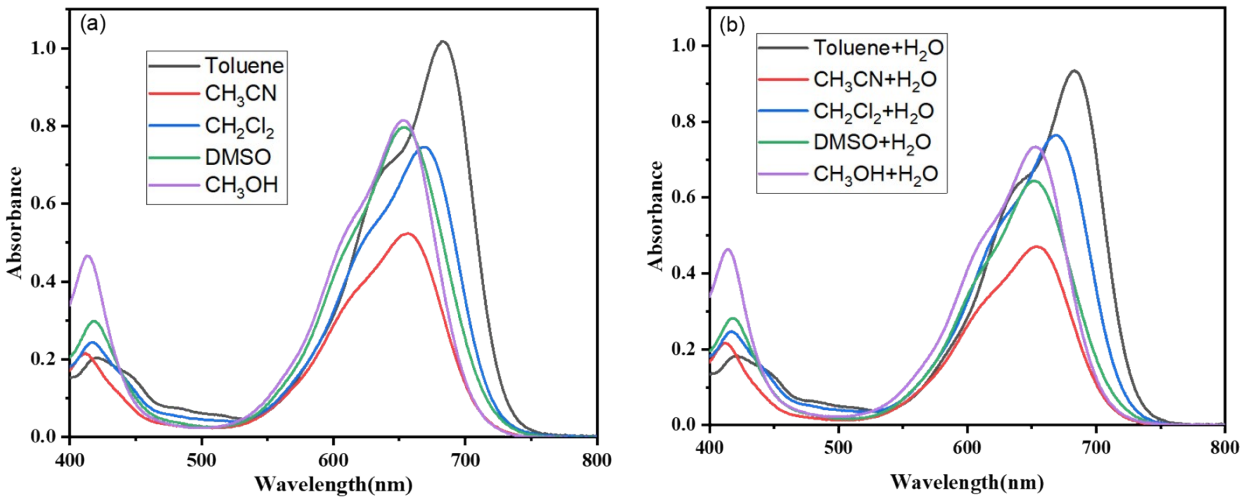


Fig. S38. Absorption spectra of compound **8** in (a) different solvents and (b) aqueous solvents (PBS buffer (pH= 7.1)).

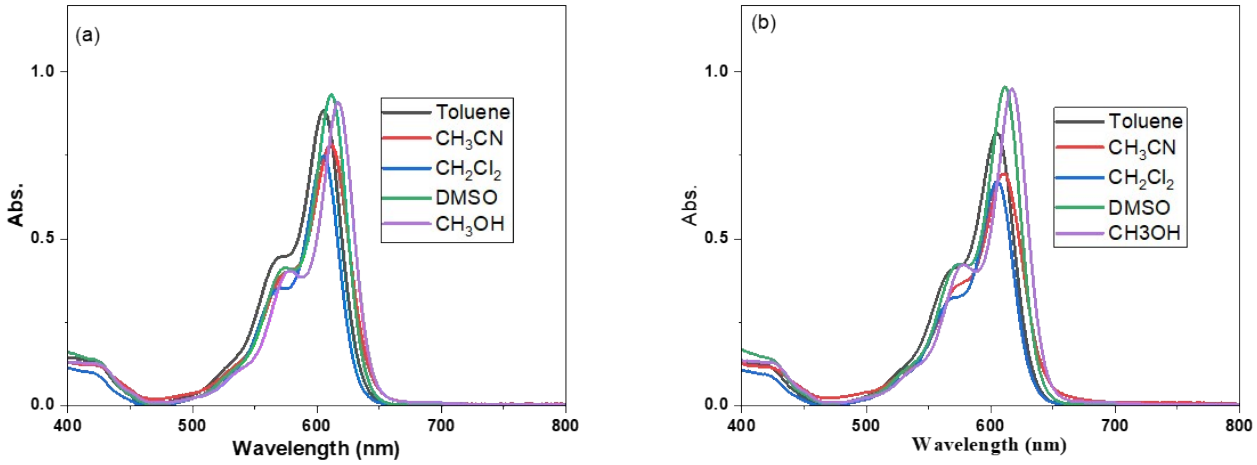


Fig. S39. Absorption spectra of compound **3** in (a) different solvents and (b) aqueous solvents (PBS buffer (pH= 7.1).

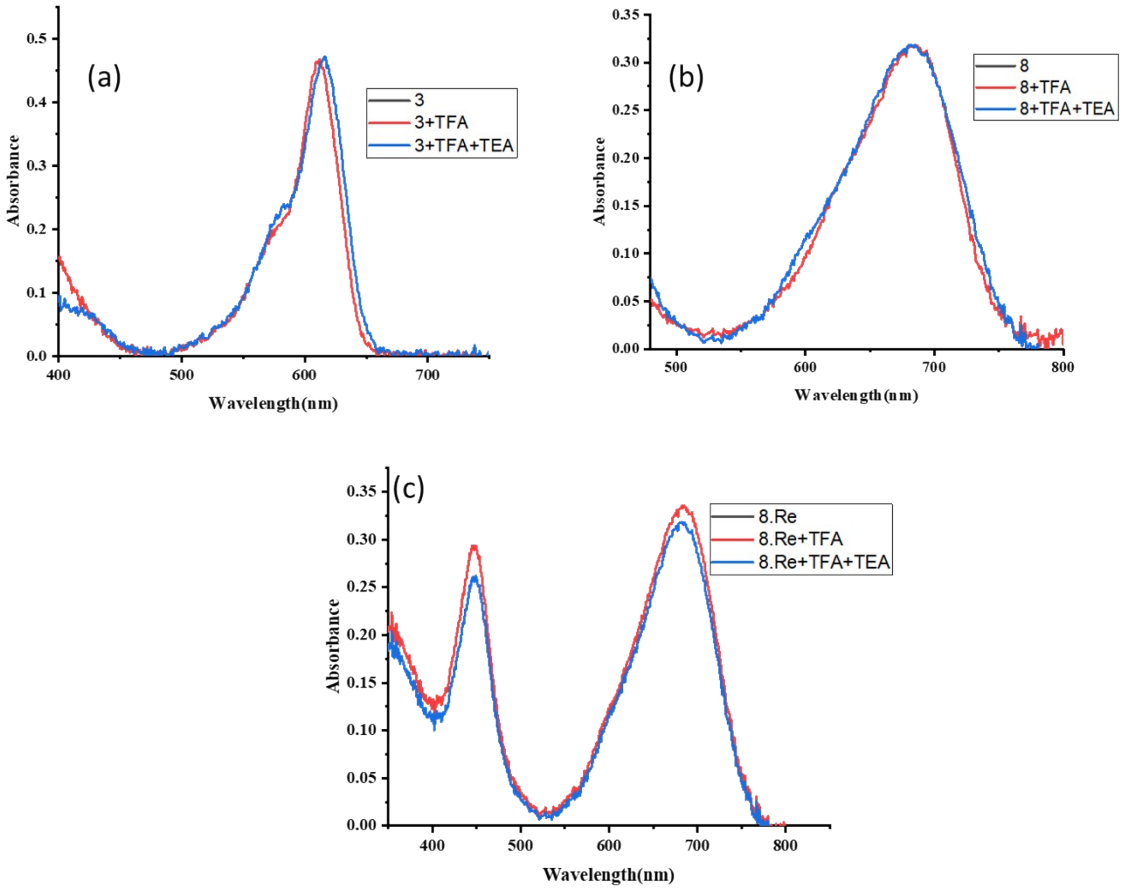


Fig. S40. Absorption spectra of compounds (a) **3**, (b) **8** and (c) **8-Re(I)** upon protonation and deprotonation in CH_2Cl_2.

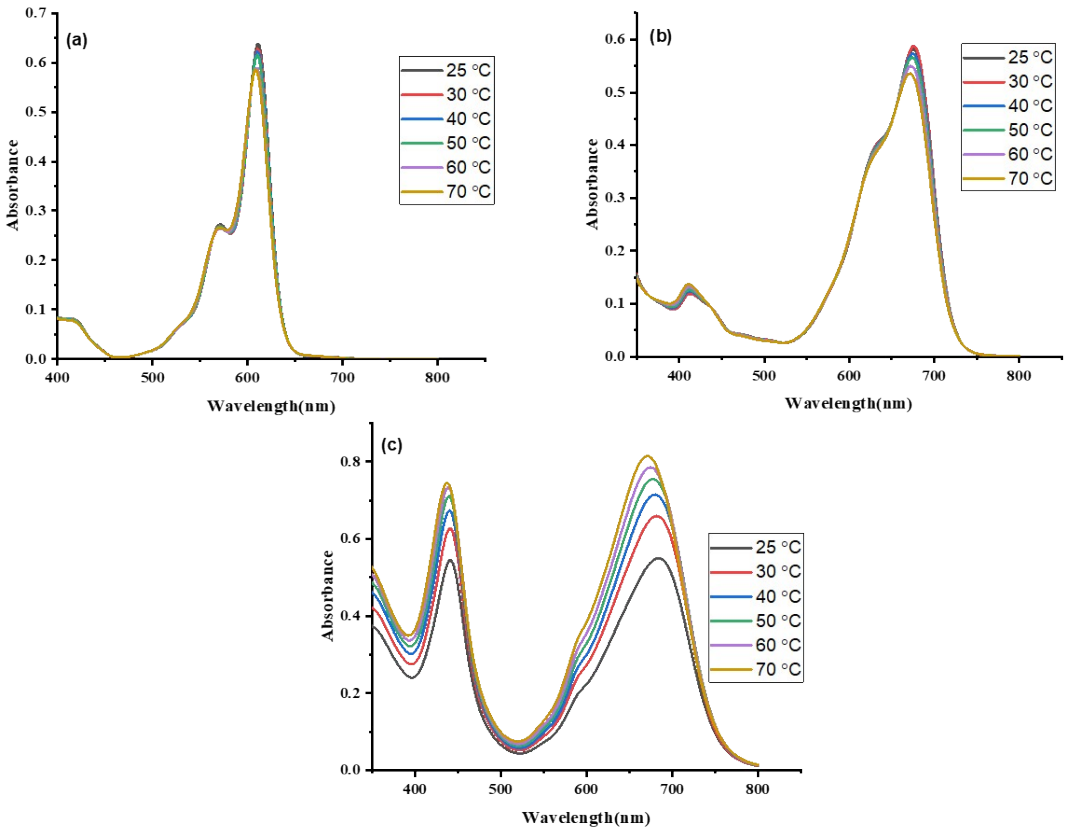


Fig. S41. Absorption spectra of compounds (a) **3**, (b) **8,** and (c) **8-Re(I)** in different temperatures in toluene.

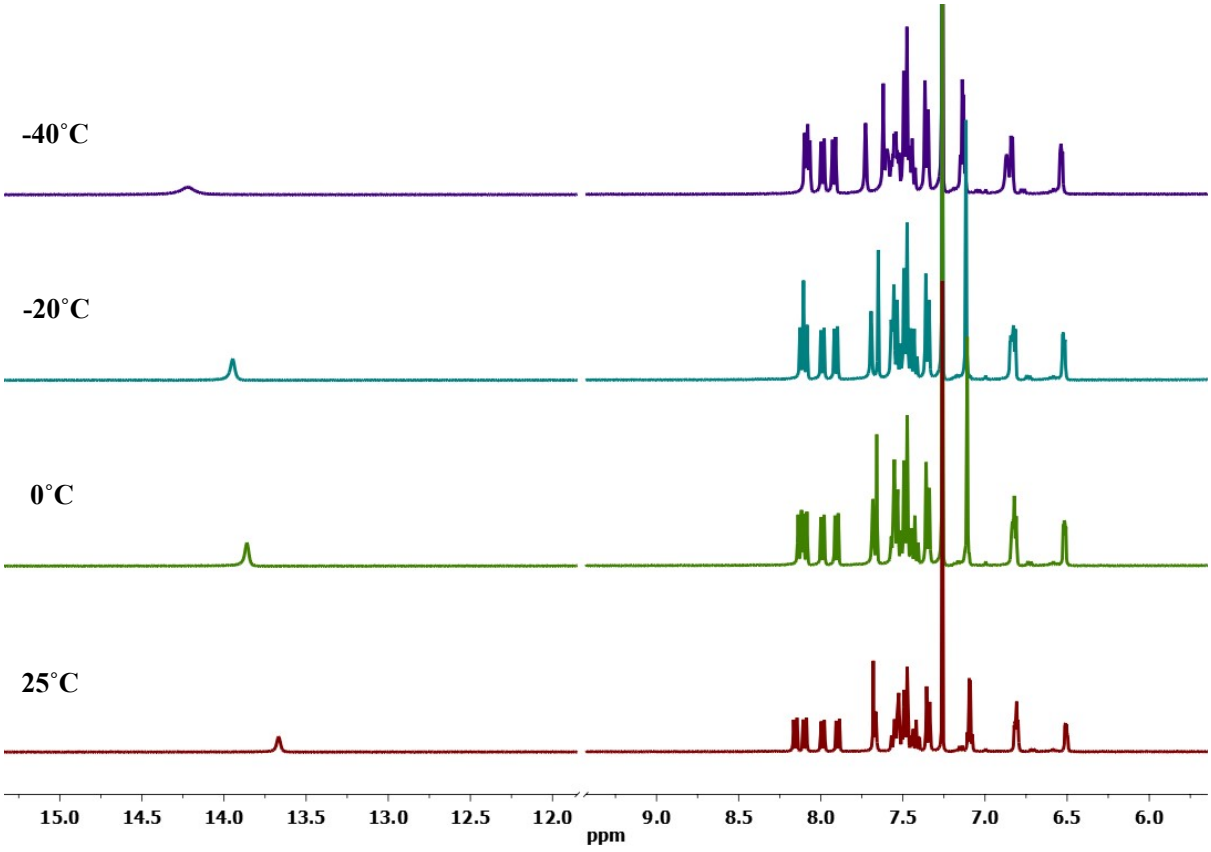


Fig. S42. ^{1}H NMR spectra of compound **8** at different temperatures in $CDCl_3$.

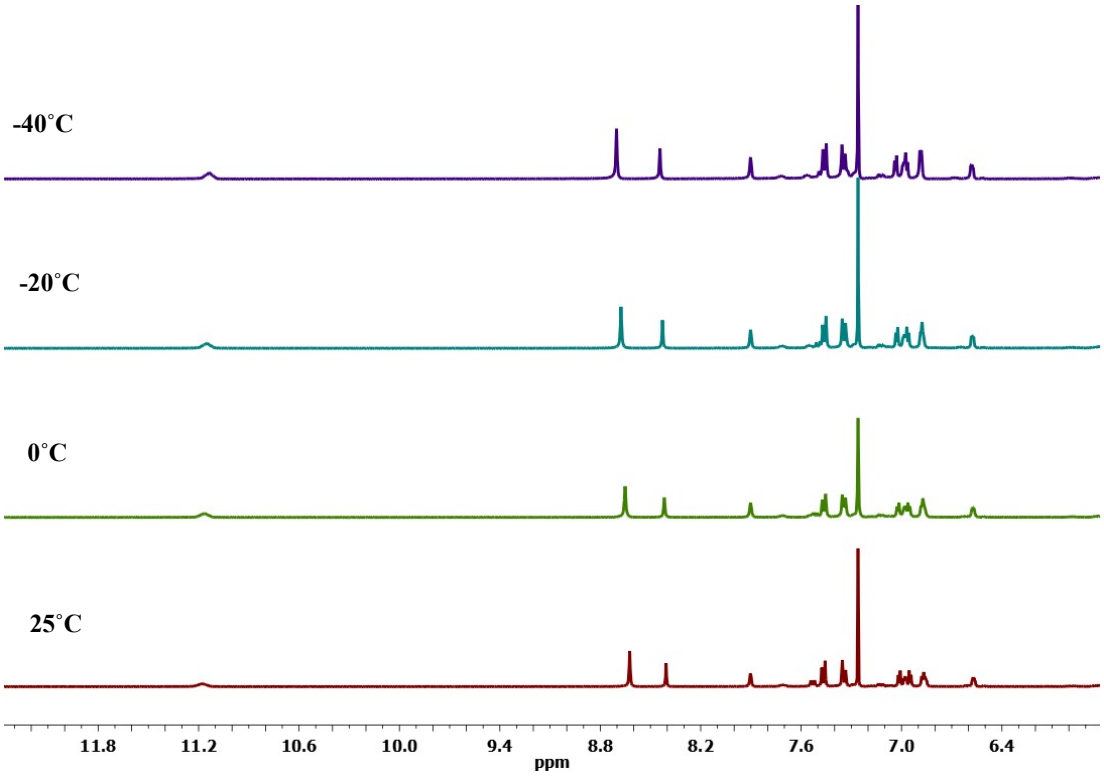


Fig. S43. ^{1}H NMR spectra of compound **3** at different temperatures in CDCl3.

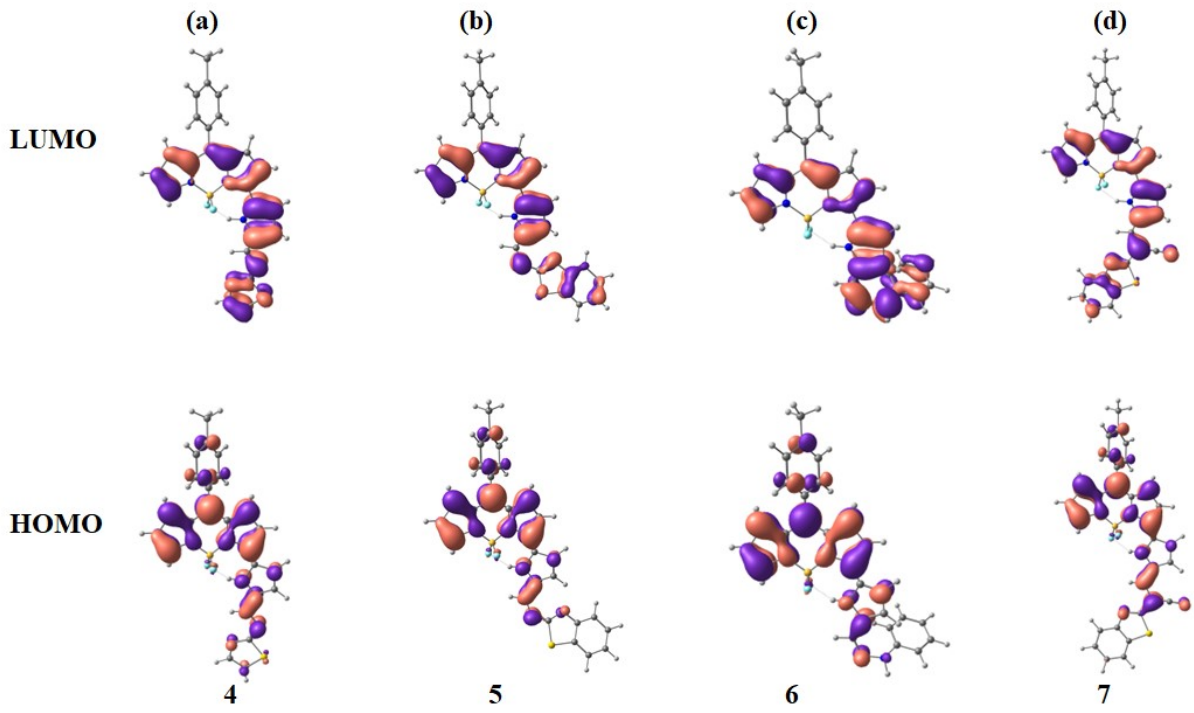


Figure S44. Frontier molecular orbitals for compounds **4, 5, 6,** and **7** at the B3LYP/6-31G(d,p) level.

Table S9. S_0 optimized geometry of compound **3** at B3LYP/6-31g (d,p) level of theory.
Total Energy (Hartree) = -1495.253802

Atom	X	Y	Z
F	1.087752701938	1.008083289066	-0.598642812152
F	0.765369185131	0.696653773064	1.639618938791
N	-0.955912751858	1.829127143771	0.369814620862
N	-0.578405470743	-0.622407776105	0.113234144682
N	6.163995769968	0.586937638951	-0.284754866712
N	2.414267209941	-1.284570030084	-0.020353612710
H	2.307873652772	-0.293445841012	-0.221294311730
N	4.922532126997	-0.002248281590	-0.206018410792
N	7.580369316280	2.255740242640	-0.552717952927
N	8.307684815091	1.092285576044	-0.331322295287
C	-1.040492088209	-2.818172037738	-0.216516145448
H	-0.871401250738	-3.874342838194	-0.368209269071
C	-0.016479438918	-1.856720239445	0.001705133691
C	1.382580504153	-2.176407973885	0.081766860346
C	-1.960127929862	-0.768014378154	-0.024555999060
C	-7.084354758791	-0.254322837758	-0.373466874703

C	**1.944237747803**	**-3.452498457147**	**0.267121177912**
H	**1.381879942268**	**-4.364833414924**	**0.402983143378**
C	**4.874549969505**	**-1.277070508944**	**-0.000615496610**
H	**5.758442211076**	**-1.907804566265**	**0.109757804705**
C	**-2.323777508771**	**1.623255127219**	**0.234299820543**
C	**-2.837016933884**	**0.326231292646**	**0.037052097671**
C	**-4.960631745902**	**-0.857010794045**	**0.650525662149**
H	**-4.398586551826**	**-1.458964361322**	**1.356501384588**
C	**-4.291636866411**	**0.123710677851**	**-0.101909793888**
C	**-0.747992930479**	**3.144365699531**	**0.575074966724**
H	**0.254132422850**	**3.524110347346**	**0.718801624262**
C	**-6.334855408853**	**-1.037204738595**	**0.515393411471**
H	**-6.836915975165**	**-1.793917393574**	**1.112267499470**
C	**6.313375151797**	**1.928775728348**	**-0.519279636270**
H	**5.463257193051**	**2.581551700873**	**-0.651638797076**
C	**3.335776169719**	**-3.303906919699**	**0.278029407002**
H	**4.078929155119**	**-4.078180438104**	**0.409982143275**
C	**-2.968922036268**	**2.875197543368**	**0.376079811198**
H	**-4.036792421814**	**3.031145935770**	**0.340152401398**
C	**-2.241396893306**	**-2.142094544111**	**-0.248963780381**
H	**-3.224423152788**	**-2.550040947272**	**-0.429374334112**
C	**-1.973914251349**	**3.829697683018**	**0.579309824078**
H	**-2.103319102358**	**4.892975799604**	**0.724544927823**
C	**-5.040840993653**	**0.913462793248**	**-0.991738067491**
H	**-4.533487114945**	**1.658919816390**	**-1.594627103724**
C	**7.452537873277**	**0.111912384800**	**-0.174527072704**
H	**7.704974471431**	**-0.919406681445**	**0.015828507668**
C	**-6.412589430022**	**0.718812461812**	**-1.126956311588**
H	**-6.972375031953**	**1.325790302479**	**-1.833482769957**
C	**3.608460481156**	**-1.942681839689**	**0.089372347113**
C	**-8.576453093175**	**-0.435045053605**	**-0.497141862724**
H	**-8.873125363857**	**-1.460932403261**	**-0.256484252177**
H	**-9.107242692335**	**0.232695286331**	**0.194281270522**
H	**-8.921152168033**	**-0.199815317290**	**-1.509356630135**
B	**0.133860708658**	**0.736436683631**	**0.407010665381**

Table S10. S_0 optimized geometry of compound **4** at B3LYP/6-31g (d,p) level of theory.

Total Energy (Hartree) = -1822.096043

Atom	X	Y	Z
C	7.114012338958	0.152882104996	0.635512623131
C	5.772749788028	0.511555864629	0.734139170644
C	4.811472872232	-0.077279777535	-0.106575171330
C	5.239611012307	-1.024724527103	-1.052670901508
C	6.584901184196	-1.370732357842	-1.149515291174
C	7.543686855214	-0.794489507513	-0.304901013418
C	8.994314785702	-1.198310069124	-0.388808424841
C	3.390999964402	0.304657123032	-0.004960398045
C	3.030232067828	1.667153824968	0.048529081123
N	1.699237143060	2.040410542747	0.188467030222
B	0.492253411670	1.088638063102	0.309268412210
N	1.032902718064	-0.360493686448	0.085755099935
C	2.392607826387	-0.679205391553	0.036349687000
C	0.335117599497	-1.528528197981	0.162437223098
C	1.248317340322	-2.618817881486	0.167650540827
C	2.519676952520	-2.093296294758	0.095575570793
C	3.801999169945	2.845383231483	-0.081479445132
C	2.921173960332	3.924394782535	-0.006053797254
C	1.634819491647	3.386951694946	0.154878640485
F	-0.117804667103	1.182909672360	1.549956600958
F	-0.447091112207	1.426493680191	-0.695642949266
C	-1.089599027819	-1.673160515921	0.228785720053
N	-2.002620164443	-0.685163805666	-0.008483528669
C	-3.275446084464	-1.179416525713	0.124406940171
C	-3.169852870841	-2.538227673742	0.468768432754
C	-1.811958120222	-2.847557387961	0.528718311564
C	-4.419836955452	-0.347436700330	-0.081591225888
N	-5.622863031053	-0.821665844352	0.035408146316
C	-6.681515614597	0.030198137637	-0.173283629997
N	-6.666048398622	1.303014238510	-0.499023040218
C	-7.939175621584	1.793867476284	-0.612820391421
C	-8.959980548679	0.911112219658	-0.377664872216
S	-8.305039722612	-0.644644777795	0.013253607164
H	7.841440975865	0.611615544785	1.299981396693
H	5.453996538276	1.235787894178	1.476021829015
H	4.514248034666	-1.462565438960	-1.730047514697

H	**6.899916325861**	**-2.092015050803**	**-1.898806774996**
H	**9.653931316105**	**-0.360615396157**	**-0.139634011277**
H	**9.213231497701**	**-2.009642939216**	**0.317973100667**
H	**9.248402946050**	**-1.557134287079**	**-1.391303461925**
H	**0.964225935936**	**-3.660351819155**	**0.206810798159**
H	**3.456374786332**	**-2.629825435029**	**0.090016407685**
H	**4.871060156675**	**2.873740654900**	**-0.231349666905**
H	**3.163677954440**	**4.975894471913**	**-0.069678670768**
H	**0.681815346662**	**3.890944107473**	**0.236295132045**
H	**-1.748499115729**	**0.255455975055**	**-0.301168895617**
H	**-4.011912386145**	**-3.189345220643**	**0.650994851865**
H	**-1.367629098409**	**-3.799992487482**	**0.780492060179**
H	**-4.236950281888**	**0.701744855082**	**-0.339695802926**
H	**-8.083094846723**	**2.835687339004**	**-0.877760685954**
H	**-10.025033689803**	**1.092561245640**	**-0.413792950791**

Table S11. S_0 optimized geometry of compound **5** at B3LYP/6-31g (d,p) level of theory. # Total Energy (hartree) = -1975.744178

Atom	**X**	**Y**	**Z**
C	**7.857463000000**	**-0.886211000000**	**0.979138000000**
C	**6.638569000000**	**-0.214398000000**	**0.962008000000**
C	**5.634507000000**	**-0.579388000000**	**0.047432000000**
C	**5.894338000000**	**-1.629887000000**	**-0.850013000000**
C	**7.120255000000**	**-2.289559000000**	**-0.831234000000**
C	**8.122103000000**	**-1.930026000000**	**0.080969000000**
C	**9.458442000000**	**-2.628707000000**	**0.079381000000**
C	**4.342361000000**	**0.129812000000**	**0.030121000000**
C	**4.313381000000**	**1.538567000000**	**0.045552000000**
N	**3.103104000000**	**2.221143000000**	**0.073808000000**
B	**1.697390000000**	**1.586792000000**	**0.086634000000**
N	**1.894086000000**	**0.044015000000**	**-0.067113000000**
C	**3.137111000000**	**-0.589487000000**	**-0.002213000000**
C	**0.934258000000**	**-0.922000000000**	**-0.035567000000**
C	**1.555401000000**	**-2.196260000000**	**0.056462000000**
C	**2.918452000000**	**-1.990185000000**	**0.082268000000**
C	**5.352481000000**	**2.496872000000**	**-0.023636000000**
C	**4.752269000000**	**3.755006000000**	**-0.023202000000**
C	**3.365450000000**	**3.542378000000**	**0.032369000000**
F	**0.963264000000**	**2.099763000000**	**-1.010024000000**

F	**1.016809000000**	**1.866361000000**	**1.260329000000**
C	**-0.486892000000**	**-0.718796000000**	**-0.085298000000**
N	**-1.110801000000**	**0.438368000000**	**-0.433458000000**
C	**-2.481957000000**	**0.278449000000**	**-0.394071000000**
C	**-2.727107000000**	**-1.053618000000**	**-0.003028000000**
C	**-1.491457000000**	**-1.669565000000**	**0.186954000000**
C	**-3.276198000000**	**1.434969000000**	**-0.705240000000**
N	**-4.545209000000**	**1.699758000000**	**-0.649862000000**
C	**-5.549258000000**	**0.823393000000**	**-0.357504000000**
N	**-5.630247000000**	**-0.463980000000**	**-0.550248000000**
C	**-6.872604000000**	**-0.950317000000**	**-0.194505000000**
C	**-7.794782000000**	**0.009905000000**	**0.301942000000**
S	**-7.043712000000**	**1.589632000000**	**0.276049000000**
C	**-7.258193000000**	**-2.297720000000**	**-0.281844000000**
C	**-8.535458000000**	**-2.663707000000**	**0.127396000000**
C	**-9.437430000000**	**-1.704448000000**	**0.622644000000**
C	**-9.076275000000**	**-0.361386000000**	**0.716896000000**
H	**8.615093000000**	**-0.603808000000**	**1.705255000000**
H	**6.441820000000**	**0.579231000000**	**1.674619000000**
H	**5.136815000000**	**-1.906792000000**	**-1.575283000000**
H	**7.307771000000**	**-3.093370000000**	**-1.538055000000**
H	**9.888431000000**	**-2.662819000000**	**1.085717000000**
H	**9.370439000000**	**-3.652272000000**	**-0.298723000000**
H	**10.172479000000**	**-2.098992000000**	**-0.565028000000**
H	**1.028169000000**	**-3.138768000000**	**0.083692000000**
H	**3.697275000000**	**-2.733686000000**	**0.159310000000**
H	**6.405738000000**	**2.266701000000**	**-0.084650000000**
H	**5.242906000000**	**4.717091000000**	**-0.068605000000**
H	**2.557526000000**	**4.260881000000**	**0.034332000000**
H	**-0.615656000000**	**1.280107000000**	**-0.717775000000**
H	**-3.708212000000**	**-1.487433000000**	**0.090739000000**
H	**-1.312859000000**	**-2.689466000000**	**0.496463000000**
H	**-2.666252000000**	**2.290046000000**	**-1.013623000000**
H	**-6.552907000000**	**-3.027614000000**	**-0.666072000000**
H	**-8.842327000000**	**-3.703339000000**	**0.064603000000**
H	**-10.430753000000**	**-2.011901000000**	**0.935208000000**
H	**-9.775619000000**	**0.375768000000**	**1.098205000000**

Table S12. S_0 optimized geometry of the compound **6** at B3LYP/6-31g (d,p) level of theory.

Total Energy (hartree) = -1540.610589

Atom	X	Y	Z
C	-6.954798000000	-0.893005000000	-0.602343000000
C	-5.774643000000	-0.154368000000	-0.613214000000
C	-4.630317000000	-0.625465000000	0.054208000000
C	-4.711019000000	-1.851820000000	0.736972000000
C	-5.898036000000	-2.579378000000	0.749128000000
C	-7.039500000000	-2.113941000000	0.081470000000
C	-8.330646000000	-2.892500000000	0.119636000000
C	-3.378082000000	0.153587000000	0.039636000000
C	-3.407543000000	1.537706000000	0.319188000000
N	-2.243227000000	2.293200000000	0.267061000000
B	-0.833601000000	1.775015000000	-0.079361000000
N	-0.942585000000	0.223857000000	-0.227326000000
C	-2.157639000000	-0.469078000000	-0.248476000000
C	0.039011000000	-0.645475000000	-0.595351000000
C	-0.540634000000	-1.917537000000	-0.864254000000
C	-1.896800000000	-1.806617000000	-0.655421000000
C	-4.459779000000	2.385988000000	0.732108000000
C	-3.915125000000	3.658444000000	0.914719000000
C	-2.547124000000	3.558882000000	0.623488000000
F	0.041974000000	2.109091000000	0.983810000000
F	-0.351879000000	2.334479000000	-1.252853000000
C	1.438942000000	-0.360874000000	-0.707583000000
N	2.066571000000	0.755769000000	-0.228317000000
C	3.414561000000	0.692892000000	-0.483965000000
C	3.653787000000	-0.514406000000	-1.163384000000
C	2.425620000000	-1.167293000000	-1.301674000000
C	4.239348000000	1.820611000000	-0.120856000000
N	5.514292000000	2.021599000000	-0.213174000000
N	6.320266000000	0.978840000000	-0.666837000000
C	6.525163000000	-0.220382000000	0.058589000000
C	5.801350000000	-0.575964000000	1.204583000000
C	6.071450000000	-1.785180000000	1.848960000000
C	7.052461000000	-2.653965000000	1.369353000000
C	7.775232000000	-2.296243000000	0.226056000000
C	7.514054000000	-1.094810000000	-0.426616000000
H	-7.823935000000	-0.522456000000	-1.139383000000
H	-5.720116000000	0.780107000000	-1.161155000000
H	-3.842211000000	-2.216781000000	1.274299000000

H	**-5.943946000000**	**-3.521384000000**	**1.289168000000**
H	**-8.928863000000**	**-2.710819000000**	**-0.779051000000**
H	**-8.142847000000**	**-3.967917000000**	**0.203119000000**
H	**-8.938132000000**	**-2.596626000000**	**0.985223000000**
H	**0.014332000000**	**-2.795268000000**	**-1.162267000000**
H	**-2.648234000000**	**-2.572267000000**	**-0.776141000000**
H	**-5.482510000000**	**2.076094000000**	**0.887574000000**
H	**-4.431450000000**	**4.554440000000**	**1.229712000000**
H	**-1.776634000000**	**4.316328000000**	**0.660725000000**
H	**1.589848000000**	**1.484820000000**	**0.295717000000**
H	**4.613878000000**	**-0.852920000000**	**-1.515580000000**
H	**2.243518000000**	**-2.113927000000**	**-1.790076000000**
H	**3.691353000000**	**2.688153000000**	**0.249498000000**
H	**7.206816000000**	**1.379367000000**	**-0.949643000000**
H	**5.042917000000**	**0.088399000000**	**1.596872000000**
H	**5.503732000000**	**-2.044174000000**	**2.738332000000**
H	**7.250978000000**	**-3.594078000000**	**1.874481000000**
H	**8.544886000000**	**-2.956773000000**	**-0.163274000000**
H	**8.070781000000**	**-0.821230000000**	**-1.319544000000**

Table S13. S_0 optimized geometry of compound **7** at B3LYP/6-31g (d,p) level of theory. # Total Energy (Hartree) = -2051.953777

Atom	**X**	**Y**	**Z**
C	**8.246871000000**	**0.635526000000**	**0.539731000000**
C	**6.879984000000**	**0.831176000000**	**0.714335000000**
C	**5.955285000000**	**0.238996000000**	**-0.164392000000**
C	**6.444702000000**	**-0.546140000000**	**-1.223201000000**
C	**7.814221000000**	**-0.728314000000**	**-1.394814000000**
C	**8.738374000000**	**-0.141438000000**	**-0.519030000000**
C	**10.221767000000**	**-0.318375000000**	**-0.724256000000**
C	**4.507560000000**	**0.443741000000**	**0.021128000000**
C	**4.003495000000**	**1.739561000000**	**0.248721000000**
N	**2.645946000000**	**1.942287000000**	**0.467568000000**
B	**1.552414000000**	**0.855463000000**	**0.487688000000**
N	**2.241804000000**	**-0.489903000000**	**0.093474000000**
C	**3.623424000000**	**-0.646773000000**	**-0.028304000000**
C	**1.678229000000**	**-1.730090000000**	**0.053086000000**
C	**2.701898000000**	**-2.704704000000**	**-0.090144000000**

C	**3.905980000000**	**-2.034443000000**	**-0.135613000000**
C	**4.638135000000**	**3.004885000000**	**0.249088000000**
C	**3.650695000000**	**3.960241000000**	**0.482937000000**
C	**2.436267000000**	**3.266074000000**	**0.606946000000**
F	**0.562262000000**	**1.196079000000**	**-0.465674000000**
F	**0.962027000000**	**0.742017000000**	**1.735561000000**
C	**0.278631000000**	**-2.035443000000**	**0.135081000000**
N	**-0.739013000000**	**-1.138326000000**	**0.018549000000**
C	**-1.956431000000**	**-1.775653000000**	**0.125355000000**
C	**-1.686308000000**	**-3.147752000000**	**0.327619000000**
C	**-0.303695000000**	**-3.306290000000**	**0.328276000000**
C	**-3.150559000000**	**-1.015576000000**	**0.019716000000**
C	**-5.555473000000**	**-0.492755000000**	**-0.053350000000**
N	**-5.388750000000**	**0.783423000000**	**-0.247480000000**
C	**-6.597563000000**	**1.441325000000**	**-0.339208000000**
C	**-7.749639000000**	**0.622861000000**	**-0.208291000000**
S	**-7.253982000000**	**-1.038620000000**	**0.040229000000**
C	**-6.750320000000**	**2.821898000000**	**-0.548111000000**
C	**-8.032130000000**	**3.353389000000**	**-0.621935000000**
C	**-9.166173000000**	**2.530056000000**	**-0.490485000000**
C	**-9.038004000000**	**1.158059000000**	**-0.282493000000**
C	**-4.454117000000**	**-1.445683000000**	**0.082630000000**
C	**-4.783110000000**	**-2.819370000000**	**0.278365000000**
N	**-5.054243000000**	**-3.941613000000**	**0.437388000000**
H	**8.946194000000**	**1.085062000000**	**1.239572000000**
H	**6.514906000000**	**1.419456000000**	**1.549237000000**
H	**5.743750000000**	**-0.991046000000**	**-1.921309000000**
H	**8.174939000000**	**-1.330569000000**	**-2.224305000000**
H	**10.758162000000**	**-0.298004000000**	**0.229972000000**
H	**10.442599000000**	**-1.263755000000**	**-1.229964000000**
H	**10.626703000000**	**0.490937000000**	**-1.346150000000**
H	**2.534852000000**	**-3.769530000000**	**-0.163599000000**
H	**4.894487000000**	**-2.458353000000**	**-0.227259000000**
H	**5.691327000000**	**3.171207000000**	**0.078297000000**
H	**3.775616000000**	**5.031965000000**	**0.547586000000**
H	**1.438811000000**	**3.647399000000**	**0.776277000000**
H	**-0.598248000000**	**-0.150864000000**	**-0.181728000000**
H	**-2.428963000000**	**-3.918708000000**	**0.461956000000**
H	**0.245816000000**	**-4.225057000000**	**0.473735000000**
H	**-3.027878000000**	**0.054211000000**	**-0.132231000000**

H	**-5.867349000000**	**3.444480000000**	**-0.647536000000**
H	**-8.162828000000**	**4.419050000000**	**-0.783129000000**
H	**-10.157523000000**	**2.968368000000**	**-0.551660000000**
H	**-9.914522000000**	**0.526465000000**	**-0.181665000000**

Table S14. S_0 optimized geometry of compound **8** at B3LYP/6-31g (d,p) level of theory. # Total Energy (Hartree) = -2681.224181

Atom	X	Y	Z
S	**4.399318000000**	**2.407884000000**	**0.349190000000**
S	**6.060992000000**	**-2.050028000000**	**-0.778180000000**
F	**-3.128950000000**	**-3.682710000000**	**-0.703645000000**
F	**-2.735201000000**	**-3.217670000000**	**1.502674000000**
N	**0.669770000000**	**-0.967077000000**	**-0.165717000000**
H	**0.867641000000**	**0.040953000000**	**-0.043633000000**
N	**2.060719000000**	**1.266375000000**	**0.211793000000**
N	**-2.983975000000**	**-1.351999000000**	**-0.041418000000**
N	**6.184541000000**	**0.344019000000**	**0.260836000000**
N	**-4.929668000000**	**-2.769725000000**	**0.611064000000**
C	**3.864019000000**	**-0.386041000000**	**-0.008946000000**
C	**1.814073000000**	**2.610047000000**	**0.384514000000**
C	**-1.818466000000**	**0.468283000000**	**-0.727613000000**
H	**-0.978974000000**	**1.068380000000**	**-1.048077000000**
C	**-1.735895000000**	**-0.891016000000**	**-0.313264000000**
C	**7.489311000000**	**-0.055683000000**	**0.057001000000**
C	**1.717366000000**	**-1.847507000000**	**-0.129247000000**
C	**-0.514421000000**	**-1.641469000000**	**-0.213943000000**
C	**3.340645000000**	**0.972732000000**	**0.167920000000**
C	**7.641478000000**	**-1.351973000000**	**-0.493945000000**
C	**2.879628000000**	**4.799596000000**	**0.631465000000**
H	**3.770670000000**	**5.416417000000**	**0.691963000000**
C	**2.971931000000**	**3.414101000000**	**0.462225000000**
C	**5.319899000000**	**-0.557390000000**	**-0.095747000000**
C	**3.098597000000**	**-1.541230000000**	**-0.084466000000**
H	**3.678519000000**	**-2.460164000000**	**-0.114375000000**
C	**-3.882793000000**	**-0.309439000000**	**-0.263003000000**
C	**-3.151366000000**	**0.822959000000**	**-0.711383000000**
H	**-3.586951000000**	**1.767700000000**	**-0.999744000000**
C	**0.540195000000**	**3.194517000000**	**0.488959000000**
H	**-0.346787000000**	**2.570567000000**	**0.451185000000**

C	**8.904065000000**	**-1.894041000000**	**-0.743685000000**
H	**9.015042000000**	**-2.887998000000**	**-1.164581000000**
C	**-0.223510000000**	**-3.024776000000**	**-0.220470000000**
H	**-0.958865000000**	**-3.808337000000**	**-0.289971000000**
C	**-6.179439000000**	**0.678402000000**	**-0.278162000000**
C	**0.452141000000**	**4.570966000000**	**0.654736000000**
H	**-0.523372000000**	**5.040033000000**	**0.738801000000**
C	**-5.264322000000**	**-0.456062000000**	**-0.051376000000**
C	**1.611304000000**	**5.367985000000**	**0.722420000000**
H	**1.516154000000**	**6.441591000000**	**0.852984000000**
C	**1.159795000000**	**-3.149976000000**	**-0.173905000000**
H	**1.735375000000**	**-4.065884000000**	**-0.183327000000**
C	**8.626276000000**	**0.708368000000**	**0.360391000000**
H	**8.504270000000**	**1.698884000000**	**0.785767000000**
C	**-5.775224000000**	**-1.688458000000**	**0.397239000000**
C	**-5.663939000000**	**-3.784349000000**	**1.100916000000**
H	**-5.195950000000**	**-4.726691000000**	**1.350253000000**
C	**9.883467000000**	**0.170059000000**	**0.108587000000**
H	**10.771615000000**	**0.750688000000**	**0.337990000000**
C	**-5.910561000000**	**1.947900000000**	**0.262269000000**
H	**-5.025934000000**	**2.086939000000**	**0.874310000000**
C	**10.021817000000**	**-1.118392000000**	**-0.438356000000**
H	**11.013553000000**	**-1.518060000000**	**-0.626415000000**
C	**-7.354175000000**	**0.505663000000**	**-1.031034000000**
H	**-7.568330000000**	**-0.466748000000**	**-1.461270000000**
C	**-7.083158000000**	**-2.072374000000**	**0.786053000000**
H	**-7.951756000000**	**-1.431242000000**	**0.760165000000**
C	**-8.221289000000**	**1.573663000000**	**-1.244933000000**
H	**-9.119567000000**	**1.424255000000**	**-1.838026000000**
C	**-6.788842000000**	**3.007465000000**	**0.050755000000**
H	**-6.574192000000**	**3.977498000000**	**0.491225000000**
C	**-7.010061000000**	**-3.393398000000**	**1.219545000000**
H	**-7.816770000000**	**-4.008613000000**	**1.592772000000**
C	**-7.954201000000**	**2.841913000000**	**-0.710615000000**
B	**-3.396593000000**	**-2.812231000000**	**0.354345000000**
C	**-8.883484000000**	**4.001847000000**	**-0.966409000000**
H	**-8.589256000000**	**4.542544000000**	**-1.875723000000**
H	**-8.861413000000**	**4.717090000000**	**-0.137759000000**
H	**-9.914260000000**	**3.660559000000**	**-1.106522000000**

Table S15. S_0 optimized geometry of the compound **8-Re(I)** at B3LYP with LANL2DZ level of theory. # Total Energy (hartree) = -3558.515832

Atom	X	Y	Z
Re	3.963025155637	-0.921477494898	-0.842243668987
S	3.742740028314	3.531310719295	0.724957627868
S	0.389468452806	-0.203140491966	2.132045859744
Cl	5.434819631032	-1.901571657329	0.675169123837
F	-2.744907421155	-0.455094732357	-0.687291442172
F	-3.484496328990	-0.670793373040	1.453756786224
O	6.277959911490	-0.708342076095	-2.963786048268
O	2.051842538778	0.337435159306	-3.055977943312
N	4.291193474086	1.077633287740	0.008424451797
O	3.255916417082	-3.734211003420	-2.081281986791
N	2.375157232915	-0.994097298420	0.659970428272
N	-1.595944781533	1.836539064910	0.279251422793
H	-1.612135954319	0.858261933107	-0.007750319458
N	-4.891102771440	-1.529892681517	-0.332201259227
N	-4.621803342276	0.919404353065	0.035452201909
C	5.526618918891	1.750311563682	0.119443146448
C	5.387520868915	3.131751770240	0.491297934521
C	0.940037074547	-1.839789948920	2.322458306932
C	6.804006494968	1.238737829795	-0.045334249313
H	6.988989345451	0.198161830479	-0.274705936806
C	3.514304544753	-2.723849018910	-1.627825726371
C	1.116597243597	-4.039329096458	3.279788301298
H	0.788276067008	-4.786902987349	3.995306687652
C	2.723480674503	-0.102974839832	-2.249397889266
C	0.480737325142	-2.788342125708	3.247196846044
H	-0.321921540306	-2.558082557586	3.940848152065
C	2.625145449648	-3.373083663200	1.478485334321
H	3.428849203091	-3.641477442544	0.809267909339
C	1.608606749535	0.078303362442	0.927831479588
C	6.499616332861	4.002282979496	0.666869439070
H	6.355267309961	5.041281978222	0.947800184167
C	1.862626476681	1.445606223606	0.461991046467
C	2.017853409990	-2.094974696822	1.444657027791
C	3.262087740369	1.852608193547	0.329083754872
C	7.914924116193	2.107338896786	0.132003911947
H	8.915854468758	1.701819035901	0.007336982284
C	5.444059118717	-0.779437505174	-2.193238107032

C	**-0.494673092104**	**2.677244860142**	**0.375550980560**
C	**2.172175545454**	**-4.322177839202**	**2.406403773607**
H	**2.655513212142**	**-5.293504169630**	**2.442897260185**
C	**-4.113612527415**	**2.172242814466**	**0.229475082430**
C	**0.911068297947**	**2.474158019870**	**0.361347892301**
H	**1.366304112662**	**3.451011506120**	**0.224091727880**
C	**-5.211410177729**	**3.117473409163**	**0.295421384568**
H	**-5.126460263842**	**4.184339167578**	**0.440305149016**
C	**-8.922204172404**	**1.045274559348**	**-1.201003327317**
H	**-8.288029214107**	**1.649938419032**	**-1.841140044127**
C	**7.760756103602**	**3.477596984810**	**0.473970826677**
H	**8.640672297828**	**4.102815512333**	**0.593615443075**
C	**-8.333601112108**	**0.072444477574**	**-0.326218307694**
C	**-6.862869261671**	**-0.088018055001**	**-0.245363212869**
C	**-2.745964431543**	**2.591151272509**	**0.349213128775**
C	**-6.286088603212**	**-1.357208471229**	**-0.413445944397**
C	**-0.997356929730**	**4.008253051383**	**0.526432938962**
H	**-0.387508558609**	**4.894905137520**	**0.641361375842**
C	**-6.007218278528**	**1.036773940688**	**-0.037226566404**
C	**-2.370083470868**	**3.954128781189**	**0.537035811612**
H	**-3.037838593900**	**4.793594481289**	**0.659630082633**
C	**-10.287620542605**	**1.165104752386**	**-1.292954690133**
H	**-10.730843742721**	**1.874841453953**	**-1.985526728572**
C	**-6.369677864806**	**2.414491411758**	**0.144089562003**
H	**-7.372424988703**	**2.815372187372**	**0.166816446884**
C	**-6.871932797921**	**-2.619672158778**	**-0.807625512494**
H	**-7.921553278344**	**-2.802571156881**	**-0.989103029379**
C	**-11.159077573917**	**0.336873214872**	**-0.495572807730**
C	**-4.630585546733**	**-2.797065104648**	**-0.646633335936**
H	**-3.616709640078**	**-3.178487530098**	**-0.655926826160**
C	**-9.185718408336**	**-0.764611413894**	**0.462838139649**
H	**-8.750819378018**	**-1.478148703506**	**1.155277724493**
C	**-5.846942607965**	**-3.511976291860**	**-0.953440689756**
H	**-5.903854615658**	**-4.549837675919**	**-1.255330711615**
B	**-3.861057594645**	**-0.456260970750**	**0.154526527002**
C	**-10.551295436750**	**-0.624748898589**	**0.398635413575**
H	**-11.194870329274**	**-1.236383250334**	**1.025382844767**
C	**-12.617860813742**	**0.464900355559**	**-0.572959019744**
H	**-12.977758970464**	**0.963264188037**	**0.355514465092**
H	**-13.121071335134**	**-0.513503659189**	**-0.536350172525**

H -12.966982064118 1.057471491675 -1.419700494259

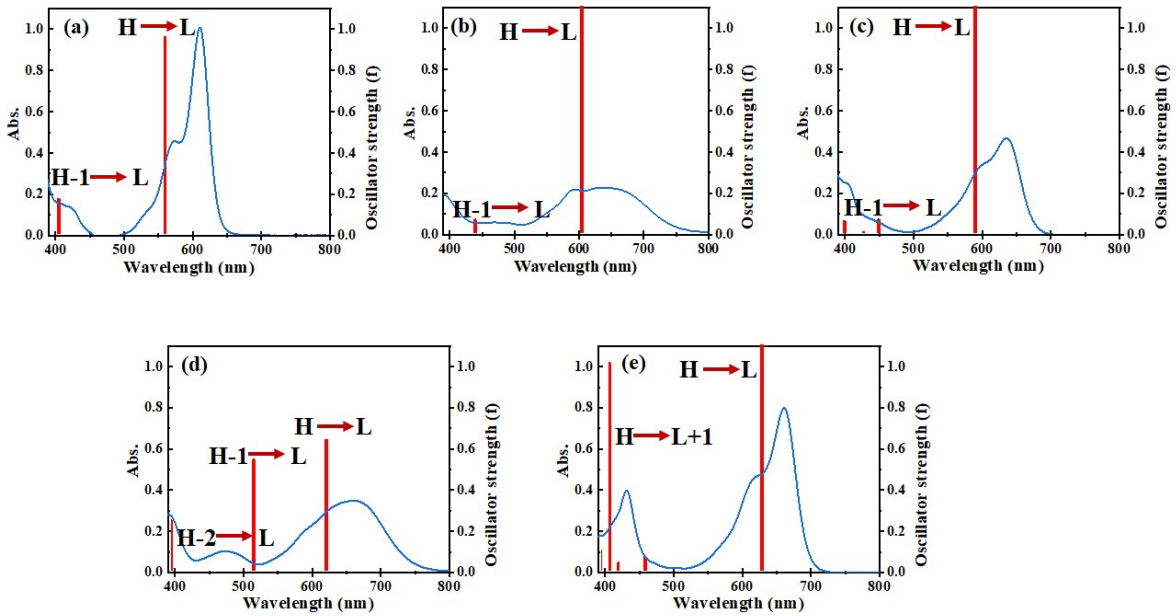


Figure S39. Calculated excitations (red vertical lines) and experimental absorption spectra (blue curve) for (a) **3,** (b) **4**, (c) **5**, (d) **6** and (e) **7**.

Table S16. Major transitions were calculated using TD-DFT studies of **3**.

Wavelength (nm)	Osc. Strength	Major contribs
554.193603666	0.8671	HOMO->LUMO (100%)
399.086467996	0.1553	H-1->LUMO (84%), HOMO->L+1 (12%)
372.079085926	0.204	H-2->LUMO (81%), HOMO->L+1 (16%)
363.121465008	0.1627	H-4->LUMO (69%), HOMO->L+1 (27%)
343.961030384	0.0001	H-3->LUMO (97%)
343.037913323	0.0628	H-5->LUMO (79%)
334.902333844	0.1915	H-8->LUMO (25%), H-6->LUMO (11%), H-5->LUMO (16%), H-4->LUMO (13%), HOMO->L+1 (21%)
333.452189264	0.1855	H-6->LUMO (70%), HOMO->L+1 (10%)
322.313133367	0.295	H-8->LUMO (72%)
316.933008722	0.0078	H-7->LUMO (94%)
279.40729484	0.0723	H-9->LUMO (19%), H-1->L+1 (61%), HOMO->L+2 (17%)
278.534794357	0.0008	H-1->L+1 (14%), HOMO->L+2 (80%)
277.475086749	0.0185	HOMO->L+3 (93%)
270.28883829	0.0245	H-9->LUMO (64%), H-1->L+1 (17%)
269.23235763	0.0018	H-3->L+1 (85%)

259.419147181	0.0005	H-10->LUMO (87%)
255.206029007	0.1106	H-2->L+1 (83%), HOMO->L+4 (12%)
250.018538036	0.0131	H-6->L+1 (44%), H-5->L+1 (11%), H-4->L+1 (10%), HOMO->L+4 (20%)
248.360796082	0.0148	H-6->L+1 (16%), H-4->L+1 (78%)
245.255856254	0.0137	H-7->L+1 (94%)
240.68992276	0.1443	H-6->L+1 (18%), HOMO->L+4 (48%)
239.578352133	0.0241	H-11->LUMO (81%)
237.772692951	0.0039	H-5->L+1 (62%)
236.236863389	0.0441	H-8->L+1 (79%)
231.3742265	0.0081	H-5->L+1 (19%), H-5->L+3 (14%), H-2->L+2 (12%), H-1->L+2 (39%)
226.409658356	0.0002	H-13->LUMO (23%), H-12->LUMO (66%)
225.028936262	0.0004	H-13->LUMO (74%), H-12->LUMO (19%)
222.245671953	0.0537	H-1->L+3 (85%)
216.626817997	0.0032	H-2->L+2 (42%), H-1->L+2 (38%)
216.403736953	0.0016	H-10->L+1 (79%)
213.832211742	0.0261	H-9->L+1 (36%), HOMO->L+5 (50%)
212.26171956	0.0383	H-9->L+1 (37%), HOMO->L+5 (23%), HOMO->L+6 (18%)
210.174760577	0.001	H-14->LUMO (81%)
209.06548127	0.004	H-15->LUMO (90%)
207.588308295	0.0322	H-16->LUMO (14%), H-4->L+2 (10%), H-2->L+3 (22%), HOMO->L+6 (32%)
207.182449096	0.0066	H-4->L+2 (19%), H-2->L+3 (12%), H-1->L+4 (16%), HOMO->L+6 (31%)
206.850619817	0.0048	H-16->LUMO (78%)
206.148999904	0.025	H-4->L+2 (53%), H-4->L+3 (24%)
204.574123044	0.0246	HOMO->L+7 (90%)
204.297707969	0.0423	H-4->L+3 (36%), H-1->L+4 (33%)
203.073005884	0.0294	H-5->L+2 (14%), H-4->L+3 (12%), H-2->L+3 (14%), H-1->L+4 (24%)
197.357920812	0.0001	H-3->L+3 (78%), H-3->L+4 (14%)
197.144526971	0.0134	H-8->L+2 (47%), H-6->L+2 (23%), H-5->L+2 (14%)
196.778442097	0.0001	H-3->L+2 (99%)
196.214776559	0.0043	H-8->L+3 (37%), H-6->L+3 (23%), H-5->L+3 (10%)
195.478499373	0.0053	H-17->LUMO (70%)
194.564360386	0.0052	H-18->LUMO (76%)
193.314508252	0.0117	H-19->LUMO (30%), H-11->L+1 (10%), H-2->L+4 (26%), HOMO->L+8 (21%)
192.674622779	0.0091	H-19->LUMO (14%), H-12->L+1 (22%), H-3->L+4 (15%)
192.563900556	0.0136	H-19->LUMO (22%), H-12->L+1 (15%), H-3->L+4 (14%)
192.193757576	0.0273	H-19->LUMO (18%), H-11->L+1 (10%), H-2->L+4 (44%), HOMO->L+8 (11%)
191.30115723	0.0004	H-12->L+1 (46%), H-3->L+4 (31%)
191.021158309	0.0072	H-11->L+1 (11%), H-8->L+2 (17%), H-8->L+3 (17%), H-6->L+2 (17%), H-6->L+3 (15%)
190.935848175	0.0053	H-11->L+1 (33%), H-8->L+2 (16%), H-6->L+2 (26%)

190.466538155	0.0122	H-11->L+1 (13%), H-8->L+3 (27%), H-6->L+3 (30%)
188.339955966	0.0008	H-7->L+2 (95%)
187.797929434	0.0021	H-7->L+3 (94%)
186.875159033	0.0162	H-3->L+7 (89%)
186.492874781	0.0211	H-21->LUMO (76%)
185.541195415	0.0637	H-4->L+4 (50%), HOMO->L+8 (16%)
185.208599872	0.1718	H-5->L+3 (29%), H-4->L+4 (11%), H-2->L+2 (19%)
183.98829598	0.2649	H-6->L+4 (45%), H-5->L+2 (10%), H-5->L+4 (18%)
182.789357078	0.3202	H-6->L+4 (13%), H-5->L+2 (26%)
181.82966403	0.0312	H-6->L+4 (20%), H-5->L+4 (44%), H-1->L+5 (14%)
181.300548376	0.0153	H-20->LUMO (29%), H-8->L+4 (16%), H-5->L+4 (23%), H-1->L+5 (19%)
180.167683405	0.0398	H-20->LUMO (51%), H-8->L+4 (20%)
179.165319883	0.0143	H-7->L+4 (89%)
178.471560403	0.0031	HOMO->L+9 (77%)
177.982218188	0.0106	H-23->LUMO (75%)
177.62269421	0.0665	H-23->LUMO (15%), H-8->L+4 (23%), H-1->L+5 (28%)
177.016594583	0.001	H-3->L+4 (23%), H-3->L+5 (10%), H-3->L+6 (56%)
174.978044529	0.0163	H-1->L+6 (69%)
174.679750081	0.1612	H-9->L+2 (66%)
174.384923644	0.2624	H-9->L+3 (65%)
174.357947675	0.0239	H-13->L+1 (84%)
173.59384085	0.0064	H-25->LUMO (10%), H-24->LUMO (72%)
173.360822467	0.0049	H-26->LUMO (17%), H-25->LUMO (58%), H-24->LUMO (11%)
172.802677406	0.0101	H-1->L+7 (86%)
171.92566458	0.159	H-2->L+5 (73%)
171.270175867	0.0384	H-22->LUMO (65%), H-4->L+5 (10%)
169.229352768	0.0221	H-22->LUMO (13%), H-4->L+5 (33%), H-1->L+8 (28%)
168.472807213	0.0156	H-9->L+4 (11%), HOMO->L+10 (41%), HOMO->L+12 (30%)
167.986604087	0.0018	H-26->LUMO (57%), H-25->LUMO (11%)
167.691237032	0.01	H-26->LUMO (10%), H-9->L+4 (32%), HOMO->L+10 (16%), HOMO->L+11 (17%)
166.58944308	0.0007	H-16->L+1 (65%), H-15->L+1 (27%)
166.016165893	0.0016	HOMO->L+10 (28%), HOMO->L+11 (10%), HOMO->L+12 (46%)
165.798599909	0.0018	H-27->LUMO (59%)
165.6878164	0.0007	H-27->LUMO (11%), H-9->L+4 (14%), HOMO->L+11 (38%)
164.925232803	0.0004	H-10->L+3 (57%), H-10->L+4 (15%)
164.714891344	0.0147	H-14->L+1 (13%), H-5->L+5 (35%), H-2->L+6 (11%)
164.673324849	0.0029	H-14->L+1 (22%), H-2->L+6 (32%)
164.594624786	0.0067	H-14->L+1 (13%), H-5->L+5 (35%), H-2->L+6 (23%)
164.42872699	0.0078	H-14->L+1 (10%), H-11->L+2 (36%), H-10->L+2 (38%)
163.985071504	0.004	H-11->L+2 (32%), H-10->L+2 (58%)

163.414470631	0.0093	H-11->L+3 (12%), H-3->L+5 (65%), H-3->L+6 (10%)
163.388628563	0.0307	H-14->L+1 (17%), H-11->L+3 (40%), H-3->L+5 (20%)
162.723863101	0.0264	H-6->L+5 (59%)
162.600087884	0.0255	H-7->L+6 (19%), H-2->L+7 (55%)
162.225644095	0.0307	H-1->L+8 (14%), HOMO->L+13 (45%)
162.077196507	0.0029	H-16->L+1 (23%), H-15->L+1 (53%)

Table S17. Major transitions calculated using TD-DFT studies of **4**.

Wavelength (nm)	**Osc. Strength**	**Major contribs**
598.234948189	1.2115	HOMO->LUMO (100%)
433.238496793	0.0602	H-1->LUMO (72%), HOMO->L+1 (27%)
384.399432666	0.8941	H-2->LUMO (36%), H-1->LUMO (14%), HOMO->L+1 (41%)
375.675523474	0.0445	H-3->LUMO (10%), H-2->LUMO (60%), HOMO->L+1 (23%)
359.770741722	0.1246	H-3->LUMO (83%)
340.428866041	0.0036	H-6->LUMO (14%), H-5->LUMO (85%)
338.061875971	0.0098	H-4->LUMO (88%)
326.945290365	0.0305	H-8->LUMO (17%), H-7->LUMO (66%)
326.437410843	0.012	H-8->LUMO (62%), H-7->LUMO (16%)
320.430550777	0.1078	H-6->LUMO (57%), H-1->L+1 (18%)
304.816700706	0.0188	H-1->L+1 (74%)
298.692314949	0.0001	H-10->LUMO (83%), H-10->L+1 (11%)
287.459583623	0.0099	HOMO->L+2 (88%)
286.675282694	0.0001	H-9->LUMO (67%), HOMO->L+3 (22%)
285.047344612	0.0197	H-9->LUMO (23%), HOMO->L+3 (70%)
273.279536715	0.0328	H-2->L+1 (92%)
268.835388912	0.0002	H-8->L+1 (12%), H-7->LUMO (10%), H-7->L+1 (68%)
261.332953254	0.0123	H-4->L+1 (62%), HOMO->L+4 (17%)
258.872077948	0.0014	H-3->L+1 (87%)
253.946281491	0.116	H-4->L+1 (24%), HOMO->L+4 (59%)
248.99924289	0.0034	H-10->LUMO (10%), H-10->L+1 (78%)
248.889276347	0.0832	H-6->L+1 (37%), H-5->L+1 (33%), HOMO->L+5 (12%)
245.183105941	0.0067	H-11->LUMO (26%), H-8->L+1 (41%), H-6->L+1 (10%)
244.26051146	0.0092	H-11->LUMO (33%), H-6->L+1 (21%), H-5->L+1 (37%)
243.24934866	0.0071	H-11->LUMO (22%), H-8->L+1 (38%)
237.918700131	0.0	H-1->L+6 (11%), HOMO->L+6 (87%)
235.250731481	0.0036	H-2->L+2 (14%), H-1->L+2 (62%)
234.534263416	0.0184	H-1->L+3 (15%), HOMO->L+5 (50%)
232.772966755	0.0456	H-1->L+3 (65%), HOMO->L+5 (12%)

232.0801771	0.0231	H-9->L+1 (88%)
227.127194644	0.0055	H-5->L+3 (11%), H-2->L+2 (35%), H-1->L+2 (19%)
224.231264377	0.0001	H-12->LUMO (95%)
219.204386436	0.0069	H-1->L+4 (27%), HOMO->L+7 (65%)
215.123352556	0.1289	H-2->L+3 (14%), H-1->L+4 (57%), HOMO->L+7 (17%)
211.429192906	0.004	H-14->LUMO (28%), H-13->LUMO (16%), H-2->L+3 (35%)
208.604682447	0.008	H-14->LUMO (26%), H-13->LUMO (18%), H-2->L+3 (15%)
208.208828193	0.0005	H-15->LUMO (79%)
207.550082884	0.0155	H-3->L+2 (79%)
207.044057599	0.0095	H-3->L+3 (83%)
205.438506424	0.0033	H-16->LUMO (92%)
203.02312632	0.0193	H-14->LUMO (15%), H-13->LUMO (27%), H-1->L+5 (39%)
200.92403295	0.0097	H-11->L+1 (33%), H-2->L+4 (46%)
200.800377378	0.0001	H-1->L+6 (74%), HOMO->L+6 (13%)
200.171447734	0.0007	H-11->L+1 (28%), H-2->L+4 (29%), H-1->L+5 (20%)
198.628953881	0.0115	H-6->L+2 (18%), H-4->L+2 (34%), H-2->L+2 (16%)
198.023019936	0.0303	H-8->L+2 (11%), H-1->L+5 (19%)
197.537151298	0.0151	H-11->L+1 (18%), H-8->L+2 (16%), H-1->L+5 (10%)
196.762827735	0.0282	H-8->L+2 (13%), H-8->L+3 (14%), H-4->L+3 (16%), HOMO->L+8 (11%)
196.295546392	0.0247	H-4->L+3 (31%), HOMO->L+8 (23%)
194.946764905	0.0121	H-8->L+3 (13%), H-6->L+3 (17%), H-5->L+3 (11%), H-3->L+4 (11%), HOMO->L+8 (16%)
194.643776904	0.007	H-18->LUMO (37%), H-8->L+3 (10%), HOMO->L+9 (13%)
193.998111426	0.0025	H-7->L+3 (11%), H-7->L+4 (40%), H-7->L+5 (25%)
193.414025884	0.0426	H-18->LUMO (20%), H-6->L+2 (10%), H-6->L+3 (17%)
193.302452467	0.0021	H-17->LUMO (86%)
193.178967315	0.0007	H-20->LUMO (11%), H-19->LUMO (69%)
192.668634539	0.0018	H-8->L+2 (30%), H-4->L+2 (36%)
191.570137534	0.0085	H-20->LUMO (67%)
191.253942049	0.0005	H-20->LUMO (11%), H-8->L+3 (12%), H-4->L+3 (16%), HOMO->L+9 (35%)
189.196412458	0.0162	H-3->L+4 (59%), HOMO->L+8 (21%)
186.973794713	0.0177	H-5->L+4 (10%), H-4->L+4 (41%), HOMO->L+9 (11%)
186.546188123	0.0302	H-21->LUMO (63%)
186.137298281	0.0553	H-4->L+4 (16%), H-1->L+7 (35%)
186.022795217	0.0011	H-10->L+4 (18%), H-10->L+5 (11%), H-7->L+2 (21%), H-7->L+3 (18%)
185.643986782	0.004	H-8->L+2 (11%), H-7->L+2 (57%), H-7->L+3 (11%)
185.469031717	0.0803	H-5->L+3 (15%), H-5->L+4 (48%)
184.489305714	0.0386	H-8->L+4 (11%), H-6->L+4 (49%)
184.01014116	0.0015	H-10->L+4 (19%), H-10->L+5 (12%), H-7->L+3 (37%)
182.514894543	0.0036	H-6->L+4 (10%), H-2->L+5 (75%)

182.302886358	0.4488	H-8->L+4 (22%), H-6->L+4 (14%), H-5->L+2 (19%)
181.781677314	0.2894	H-6->L+2 (24%), H-5->L+3 (18%), H-5->L+4 (21%)
180.327529652	0.0002	H-9->L+6 (74%)
180.039487421	0.0175	H-9->L+3 (37%), H-9->L+4 (20%), H-7->L+6 (10%)
178.466422461	0.2932	H-8->L+4 (17%), H-5->L+2 (16%), H-1->L+7 (14%)
178.163806599	0.0012	H-24->LUMO (22%), H-23->LUMO (37%), H-22->LUMO (22%)
177.928579852	0.0766	H-9->L+2 (82%)
177.541302249	0.0006	H-12->L+1 (89%)
177.462524887	0.0012	H-10->L+2 (13%), H-7->L+4 (26%), H-7->L+5 (38%)
177.409199285	0.0004	H-10->L+2 (86%)
176.623207562	0.0001	H-10->L+3 (80%), H-10->L+5 (11%)
176.437211669	0.0	H-9->L+3 (42%), H-9->L+4 (10%), H-7->L+6 (10%)
176.23657519	0.0007	H-24->LUMO (20%), H-22->LUMO (46%), H-21->LUMO (11%)
175.619979337	0.0006	H-9->L+6 (16%), H-2->L+6 (62%)
175.532956284	0.0064	H-3->L+5 (24%), H-2->L+7 (45%)
174.82260718	0.0029	H-25->LUMO (14%), H-3->L+5 (40%), H-2->L+7 (26%)
174.505190801	0.0557	H-25->LUMO (19%), H-4->L+5 (52%)
174.237883319	0.0323	H-25->LUMO (36%), H-4->L+5 (14%), H-3->L+5 (15%)
173.360822467	0.0006	H-26->LUMO (78%)
172.882192275	0.0398	H-9->L+4 (18%), H-7->L+6 (37%)
172.624636972	0.018	H-13->L+1 (10%), H-3->L+7 (23%), H-1->L+8 (24%)
171.966202963	0.049	H-13->L+1 (20%), H-3->L+7 (10%), HOMO->L+11 (17%)
170.991453492	0.0009	HOMO->L+11 (46%)
170.718338055	0.0145	H-24->LUMO (29%), H-23->LUMO (27%), HOMO->L+11 (10%)
170.500004142	0.0026	H-17->L+1 (86%)
170.286905482	0.0014	H-13->L+1 (20%), H-9->L+4 (11%), H-6->L+5 (16%), H-5->L+5 (17%)
169.750671576	0.0001	H-10->L+4 (44%), H-10->L+5 (44%)
169.321797515	0.0042	HOMO->L+10 (85%)
168.931904967	0.042	H-16->L+1 (15%), H-14->L+1 (15%), H-11->L+2 (35%), H-11->L+3 (16%)
168.816896113	0.0211	H-16->L+1 (45%), H-11->L+2 (10%), H-1->L+9 (10%)
168.729594061	0.0108	H-16->L+1 (17%), H-10->L+6 (31%), H-1->L+9 (24%)
168.468228837	0.0492	H-27->LUMO (10%), H-14->L+1 (10%), H-11->L+2 (35%), H-11->L+3 (28%)

Table S18. Major transitions calculated using TD-DFT studies of **5**.

Wavelength (nm)	**Osc. Strength**	**Major contribs**
584.307427363	1.3044	HOMO->LUMO (99%)
443.624563519	0.059	H-1->LUMO (91%)
421.686256079	0.0046	H-2->LUMO (99%)

393.775624126	0.0538	H-3->LUMO (28%), HOMO->L+1 (64%)
386.231559803	0.5846	H-3->LUMO (66%), HOMO->L+1 (20%)
365.217959857	0.018	H-5->LUMO (14%), H-4->LUMO (83%)
346.169848705	0.0072	H-6->LUMO (22%), H-5->LUMO (59%)
344.28577422	0.0121	H-7->LUMO (57%), H-6->LUMO (39%)
334.829979238	0.0369	H-7->LUMO (34%), H-6->LUMO (30%), H-5->LUMO (12%)
331.313647085	0.0441	H-8->LUMO (44%), H-1->L+1 (39%)
326.523381033	0.0834	H-9->LUMO (22%), H-8->LUMO (40%), H-1->L+1 (20%)
315.7947913	0.0132	H-2->L+1 (90%)
312.625615906	0.0441	H-9->LUMO (58%), H-1->L+1 (15%)
303.704176495	0.0599	H-10->LUMO (71%), H-1->L+1 (16%)
282.984942853	0.0001	H-3->L+1 (76%)
280.551655267	0.0059	HOMO->L+2 (91%)
279.703550911	0.0034	HOMO->L+3 (86%)
267.201553872	0.0306	H-9->L+1 (11%), H-6->L+1 (51%), H-5->L+1 (18%)
265.042418633	0.0553	H-9->L+1 (26%), H-4->L+1 (32%), H-3->L+1 (11%)
261.608661642	0.052	H-11->LUMO (70%), HOMO->L+4 (17%)
260.072143587	0.0571	H-11->LUMO (19%), H-9->L+1 (18%), H-4->L+1 (13%), HOMO->L+4 (29%)
257.897437363	0.1075	H-10->L+1 (16%), H-9->L+1 (18%), H-6->L+1 (12%), HOMO->L+4 (25%)
257.645552995	0.0059	H-10->L+1 (12%), H-5->L+1 (38%), H-4->L+1 (31%)
255.416326093	0.019	HOMO->L+5 (70%)
249.927820134	0.0736	H-10->L+1 (39%), H-6->L+1 (16%), H-5->L+1 (17%)
248.06761307	0.0157	H-12->LUMO (75%)
245.06679517	0.0086	H-8->L+1 (30%), H-7->L+1 (58%)
244.03935245	0.0024	H-8->L+1 (55%), H-7->L+1 (30%)
239.370208148	0.0037	H-1->L+7 (13%), HOMO->L+7 (75%)
236.719476501	0.0152	H-1->L+3 (20%), HOMO->L+6 (57%)
236.308904668	0.0353	H-1->L+3 (25%), H-1->L+5 (11%)
234.929783064	0.0037	H-3->L+2 (16%), H-1->L+2 (60%)
232.768596662	0.0502	H-2->L+4 (12%), H-1->L+3 (27%), H-1->L+5 (16%)
228.96434536	0.0045	H-7->L+3 (13%), H-3->L+2 (25%), H-1->L+2 (19%)
227.58997928	0.0179	H-15->LUMO (11%), H-13->LUMO (67%)
227.289580033	0.0011	H-13->LUMO (11%), H-1->L+4 (37%)
224.247486864	0.0043	H-15->LUMO (83%), H-13->LUMO (13%)
221.641775885	0.0033	H-2->L+2 (95%)
221.19889567	0.0261	H-2->L+3 (68%), H-1->L+5 (16%)
220.021282696	0.0013	H-2->L+7 (91%)
219.06882644	0.0487	H-11->L+1 (48%), H-2->L+3 (10%), H-2->L+4 (13%)
216.869324842	0.0001	H-14->LUMO (96%)
216.298028667	0.0888	H-3->L+2 (12%), H-3->L+3 (49%), HOMO->L+8 (27%)

214.483259544	0.0037	H-11->L+1 (18%), H-3->L+3 (11%), HOMO->L+8 (33%)
213.787966018	0.065	H-11->L+1 (13%), H-2->L+4 (37%), H-1->L+5 (19%), HOMO->L+8 (13%)
212.250818318	0.1415	H-16->LUMO (21%), H-2->L+5 (23%), H-1->L+6 (11%), H-1->L+7 (12%)
211.533803679	0.001	H-16->LUMO (11%), H-1->L+7 (60%), HOMO->L+7 (11%)
210.460173842	0.071	H-16->LUMO (51%), H-2->L+5 (10%)
209.012614866	0.001	H-17->LUMO (91%)
207.981804325	0.0743	H-4->L+2 (25%), H-4->L+3 (14%), H-3->L+2 (12%), H-3->L+4 (19%)
207.557031911	0.0973	H-4->L+2 (26%), H-3->L+4 (20%), H-1->L+6 (10%)
206.936931289	0.0088	H-5->L+2 (12%), H-5->L+3 (10%), H-4->L+2 (22%), H-4->L+3 (34%)
206.104450117	0.0269	H-18->LUMO (48%), H-3->L+4 (11%), H-1->L+6 (15%)
205.974337994	0.051	H-18->LUMO (40%), H-3->L+4 (17%), H-1->L+6 (19%)
204.553872191	0.0163	H-7->L+3 (13%), H-5->L+2 (38%), H-5->L+3 (12%)
202.953336082	0.0643	H-12->L+1 (23%), H-2->L+6 (51%)
201.626541684	0.0027	H-5->L+3 (29%), H-4->L+3 (10%), HOMO->L+9 (26%)
200.83941006	0.0409	H-12->L+1 (35%), H-6->L+3 (10%)
200.693115692	0.0696	H-12->L+1 (16%), H-6->L+3 (15%), HOMO->L+9 (15%)
198.384231263	0.0013	H-8->L+2 (16%), H-6->L+2 (19%), H-6->L+3 (15%), HOMO->L+9 (16%)
197.962945892	0.0134	H-8->L+2 (11%), H-4->L+4 (26%), H-3->L+5 (11%)
197.474226347	0.0009	H-8->L+2 (15%), H-8->L+3 (11%), H-6->L+2 (14%), H-6->L+3 (14%), H-4->L+4 (12%)
197.113184439	0.0661	H-3->L+5 (52%)
196.391935835	0.0004	H-20->LUMO (13%), H-9->L+4 (15%), H-8->L+3 (17%)
195.611114987	0.0082	H-20->LUMO (38%), H-19->LUMO (14%)
195.342985682	0.0243	H-8->L+3 (11%), H-6->L+4 (13%), H-5->L+4 (13%), HOMO->L+10 (19%)
194.842602128	0.0396	H-8->L+2 (11%), H-8->L+3 (15%)
194.092257255	0.0048	H-8->L+2 (36%), H-8->L+3 (14%), H-6->L+2 (20%)
193.858579355	0.002	H-22->LUMO (73%)
193.076684594	0.0024	H-23->LUMO (21%), H-20->LUMO (11%), H-19->LUMO (49%)
192.342837438	0.0007	H-8->L+3 (14%), H-6->L+3 (10%), H-6->L+4 (17%), H-5->L+4 (27%)
191.917082817	0.0034	H-23->LUMO (56%), H-19->LUMO (11%)
191.878471295	0.0012	H-10->L+5 (30%), H-9->L+5 (23%)
189.82789756	0.0121	H-13->L+1 (23%), HOMO->L+10 (16%)
189.63626952	0.0388	H-3->L+6 (52%)
188.919657787	0.0279	H-6->L+4 (25%), HOMO->L+10 (19%)
188.801707065	0.0009	H-14->L+1 (85%)
187.718315486	0.028	H-7->L+3 (15%), H-7->L+4 (41%)
187.29295902	0.0193	H-8->L+4 (27%), H-1->L+8 (38%)
186.976614405	0.0472	H-25->LUMO (32%), H-24->LUMO (30%)
186.877975751	0.0031	H-9->L+5 (21%), H-5->L+5 (15%), H-4->L+5 (44%)
186.431181601	0.0041	H-13->L+1 (15%), H-6->L+5 (14%)
185.877774298	0.0152	H-6->L+5 (52%), H-4->L+5 (10%)

184.695426734	0.1414	H-21->LUMO (11%), H-9->L+2 (10%), H-8->L+4 (17%)
184.593682834	0.0447	H-21->LUMO (25%), H-9->L+2 (18%)
184.33296117	0.1946	H-9->L+2 (33%), H-8->L+4 (11%), H-7->L+2 (11%), H-1->L+8 (13%)
184.212455259	0.0053	H-21->LUMO (42%), H-3->L+7 (22%)
183.669401831	0.004	H-4->L+5 (10%), H-3->L+7 (30%)
183.080865628	0.0293	H-9->L+2 (17%), H-9->L+3 (12%), H-9->L+4 (10%), H-5->L+5 (12%)
182.827092844	0.1352	H-9->L+2 (13%), H-9->L+3 (24%)
182.152900144	0.0059	H-6->L+5 (13%), H-5->L+5 (33%)
181.483661478	0.0435	H-10->L+2 (17%), H-10->L+3 (19%), H-4->L+6 (16%)
180.858887302	0.0886	H-10->L+2 (52%), H-10->L+3 (18%)
180.406246653	0.0658	H-4->L+6 (19%), H-1->L+9 (27%)
179.953254103	0.2412	H-7->L+2 (13%), H-1->L+9 (17%)
179.747151967	0.0216	H-25->LUMO (20%), H-24->LUMO (23%), H-10->L+3 (10%)
179.546721424	0.0421	H-2->L+8 (56%)
179.53112223	0.1054	H-6->L+6 (14%), H-2->L+8 (41%)
178.842271316	0.0096	H-9->L+4 (11%), H-6->L+6 (35%)
177.989883448	0.0366	H-10->L+7 (15%), H-9->L+7 (35%), H-1->L+9 (13%)

Table S19. Major transitions calculated using TD-DFT studies of **6**.

Wavelength (nm)	**Osc. Strength**	**Major contribs**
614.817975861	0.5789	HOMO->LUMO (93%)
509.258987153	0.4902	H-1->LUMO (92%)
389.092085398	0.2229	H-2->LUMO (88%)
364.445011794	0.1296	H-4->LUMO (30%), H-3->LUMO (61%)
357.231085983	0.0986	H-5->LUMO (36%), H-4->LUMO (38%), H-3->LUMO (10%), HOMO->L+1 (12%)
350.485351271	0.0963	H-4->LUMO (10%), H-3->LUMO (22%), HOMO->L+1 (49%)
336.977666981	0.0073	H-7->LUMO (17%), H-5->LUMO (43%), H-4->LUMO (14%), H-1->L+1 (12%)
333.84725352	0.0129	H-7->LUMO (48%), H-6->LUMO (37%)
329.16740034	0.0136	H-7->LUMO (32%), H-6->LUMO (51%)
323.119525194	0.0136	H-8->LUMO (87%)
302.039496729	0.0014	H-9->LUMO (91%)
301.386049424	0.3007	H-1->L+1 (61%), HOMO->L+1 (16%)
291.193088008	0.0018	HOMO->L+2 (93%)
287.693041146	0.0821	HOMO->L+3 (90%)
278.678788519	0.0183	HOMO->L+4 (85%)
258.058472291	0.0127	H-1->L+2 (74%), HOMO->L+5 (11%)

257.897437363	0.0843	H-1->L+2 (18%), H-1->L+4 (14%), HOMO->L+5 (44%)
256.855589418	0.012	H-1->L+3 (72%)
253.551592082	0.0292	H-10->LUMO (15%), H-2->L+1 (55%), HOMO->L+5 (10%)
252.66801103	0.0348	H-10->LUMO (46%), H-1->L+4 (20%), HOMO->L+6 (10%)
248.201695618	0.1099	H-10->LUMO (15%), H-2->L+1 (14%), H-1->L+4 (35%), HOMO->L+5 (24%)
242.137709968	0.0139	H-3->L+1 (41%), HOMO->L+6 (33%)
238.642247011	0.0048	H-3->L+1 (36%), H-2->L+1 (15%), HOMO->L+6 (29%)
234.016332293	0.0252	H-11->LUMO (12%), H-4->L+1 (11%), H-2->L+2 (11%), H-1->L+5 (36%)
233.835375905	0.0655	H-11->LUMO (61%)
233.619477704	0.0214	H-7->L+3 (13%), H-2->L+2 (31%), H-1->L+5 (23%)
227.824172676	0.0155	H-5->L+1 (18%), H-4->L+1 (59%)
227.381284524	0.078	H-9->L+1 (20%), H-6->L+1 (27%), H-1->L+5 (10%)
226.157734144	0.0061	H-6->L+1 (20%), H-5->L+1 (25%), H-1->L+6 (29%)
223.29435932	0.0532	H-9->L+1 (30%), H-2->L+3 (17%), H-1->L+6 (17%)
222.301459509	0.0047	H-13->LUMO (86%)
221.867851924	0.0385	H-6->L+1 (14%), H-5->L+1 (10%), H-2->L+3 (28%), H-1->L+6 (28%)
221.218629362	0.0603	H-13->LUMO (10%), H-9->L+1 (12%), H-2->L+3 (23%), HOMO->L+7 (27%)
218.543666735	0.0076	H-8->L+1 (26%), H-5->L+1 (13%), H-2->L+3 (15%), HOMO->L+7 (23%)
217.302637781	0.0018	H-7->L+1 (11%), H-4->L+2 (19%), H-3->L+2 (11%), H-2->L+2 (43%)
214.260866506	0.0222	H-8->L+1 (42%), H-7->L+1 (17%), HOMO->L+7 (20%)
212.26171956	0.0098	H-8->L+1 (13%), H-7->L+1 (60%)
208.653831158	0.0522	H-2->L+4 (51%)
208.523988382	0.0149	H-5->L+2 (50%), H-4->L+2 (23%), H-2->L+4 (14%)
207.946921511	0.0147	H-14->LUMO (42%), H-4->L+3 (20%)
206.874779771	0.019	H-14->LUMO (35%), H-5->L+3 (24%), H-4->L+3 (24%)
206.186710923	0.0049	H-16->LUMO (80%)
205.129203223	0.0103	H-5->L+3 (19%), H-3->L+3 (51%)
204.946100589	0.0016	H-12->LUMO (97%)
203.412837991	0.0067	H-17->LUMO (81%)
203.309435436	0.0022	H-17->LUMO (14%), H-5->L+2 (12%), H-4->L+2 (13%), H-3->L+2 (50%)
201.201183039	0.0126	H-5->L+3 (13%), H-4->L+3 (17%), H-3->L+3 (11%), H-1->L+7 (34%)
200.391448356	0.0052	H-7->L+2 (10%), H-5->L+3 (16%), H-1->L+7 (48%)
199.707154957	0.0144	H-2->L+5 (52%)
197.918704125	0.0042	H-8->L+2 (53%), H-6->L+2 (34%)
197.830279889	0.017	H-9->L+4 (20%), H-3->L+4 (10%), H-2->L+4 (13%), H-2->L+5 (22%)
196.806554196	0.0074	H-8->L+3 (25%), H-6->L+3 (21%), HOMO->L+8 (26%)
195.731549969	0.0599	H-15->LUMO (31%), H-6->L+4 (15%), H-3->L+4 (22%)
195.392241643	0.0599	H-15->LUMO (20%), HOMO->L+8 (36%)
195.072521181	0.0186	H-15->LUMO (23%), H-6->L+3 (16%), H-6->L+4 (10%), H-3->L+4 (15%), HOMO->L+8 (14%)

194.025434676	0.0009	H-8->L+2 (36%), H-6->L+2 (52%)
193.227137867	0.043	H-19->LUMO (20%), H-8->L+3 (28%), H-6->L+3 (23%)
192.522038839	0.0073	H-19->LUMO (52%), H-8->L+3 (16%), H-6->L+3 (10%)
191.56421775	0.0116	H-20->LUMO (13%), H-6->L+4 (20%), H-2->L+6 (27%)
191.487293835	0.0015	H-21->LUMO (11%), H-20->LUMO (61%)
190.165638535	0.0017	H-21->LUMO (15%), H-4->L+4 (41%)
189.77559697	0.009	H-21->LUMO (60%), H-20->LUMO (15%), H-4->L+4 (11%)
189.184864826	0.001	H-18->LUMO (91%)
188.821834565	0.0325	H-4->L+4 (15%), H-3->L+5 (25%), H-3->L+6 (15%), H-2->L+6 (19%)
187.991559031	0.0566	H-10->L+1 (52%)
187.072534571	0.0439	H-5->L+4 (60%)
186.613574877	0.08	H-6->L+4 (24%), H-3->L+4 (11%), H-3->L+5 (16%)
186.1400928	0.0855	H-9->L+2 (54%), H-7->L+3 (16%)
185.302714152	0.0216	H-23->LUMO (34%), H-22->LUMO (38%)
184.412471758	0.0135	H-9->L+3 (45%), H-6->L+5 (16%)
183.939163285	0.0541	H-4->L+5 (56%)
183.441133059	0.0337	H-6->L+5 (44%)
182.905309374	0.1962	H-9->L+2 (35%), H-7->L+3 (28%)
182.367241803	0.268	H-7->L+2 (14%), H-5->L+5 (29%)
181.997817234	0.1865	H-7->L+2 (18%), H-5->L+5 (10%), H-1->L+8 (16%)
180.821959561	0.0262	H-8->L+4 (17%), HOMO->L+10 (29%), HOMO->L+11 (13%)
180.70863287	0.0381	H-8->L+4 (12%), H-7->L+4 (21%), H-2->L+7 (10%), HOMO->L+10 (10%)
180.110103449	0.0301	H-7->L+4 (49%), H-1->L+8 (12%)
179.593535275	0.0769	H-6->L+5 (10%), H-6->L+6 (24%), H-1->L+8 (15%)
179.541521392	0.1234	H-2->L+7 (22%), H-1->L+8 (26%)
178.494684805	0.0031	H-8->L+4 (16%), H-6->L+6 (13%), HOMO->L+11 (21%)
178.081918089	0.0244	H-26->LUMO (15%), H-23->LUMO (34%), H-22->LUMO (30%)
177.829051523	0.0426	H-8->L+4 (16%), H-2->L+7 (21%)
176.505029628	0.009	H-6->L+6 (19%), H-4->L+6 (45%)
175.749430176	0.0104	H-11->L+1 (24%), HOMO->L+10 (16%), HOMO->L+12 (10%)
175.483267536	0.0243	H-26->LUMO (20%), H-24->LUMO (25%)
175.341808814	0.01	H-7->L+5 (59%)
175.133758528	0.0104	H-26->LUMO (32%), H-8->L+5 (14%)
174.48308848	0.014	H-26->LUMO (10%), H-24->LUMO (46%)
174.277069821	0.1026	H-9->L+5 (12%), H-8->L+5 (33%)
173.579258851	0.0339	H-5->L+6 (64%)
173.014879798	0.0011	HOMO->L+11 (11%), HOMO->L+12 (51%)
171.830355502	0.2736	H-9->L+4 (11%), H-9->L+5 (20%)
171.495232118	0.0304	H-10->L+2 (14%), H-4->L+7 (21%), H-3->L+7 (16%), HOMO->L+9 (16%)
171.237059612	0.0407	H-27->LUMO (47%)

171.133063275	0.0408	H-10->L+2 (12%), HOMO->L+9 (52%)
171.074030704	0.1183	H-10->L+2 (39%), H-3->L+7 (14%)
170.380509574	0.1152	H-10->L+3 (54%)
169.764617381	0.157	H-9->L+6 (14%), HOMO->L+14 (47%)
169.701879294	0.0253	H-25->LUMO (36%)

Table S20. Major transitions calculated using TD-DFT studies of **7**.

Wavelength (nm)	**Osc. Strength**	**Major contribs**
622.723219549	1.287	HOMO->LUMO (100%)
452.629209303	0.0614	H-1->LUMO (56%), HOMO->L+1 (43%)
413.652931012	0.0358	H-2->LUMO (87%)
401.386231384	0.9165	H-2->LUMO (11%), H-1->LUMO (32%), HOMO->L+1 (46%)
386.99105129	0.0927	H-3->LUMO (92%)
366.156324421	0.0747	H-4->LUMO (85%)
347.78174758	0.0047	H-7->LUMO (10%), H-6->LUMO (64%), H-5->LUMO (22%)
340.765701991	0.0156	H-7->LUMO (42%), H-6->LUMO (29%), H-5->LUMO (17%)
335.682125388	0.1049	H-7->LUMO (22%), H-5->LUMO (25%), H-1->L+1 (33%)
331.180898609	0.003	H-8->LUMO (53%), H-7->LUMO (23%), H-1->L+1 (12%)
323.752331868	0.0466	H-8->LUMO (27%), H-1->L+1 (46%)
318.93860424	0.0127	H-2->L+1 (88%)
307.264238835	0.0002	H-9->LUMO (89%), H-9->L+1 (10%)
292.153713682	0.0082	H-3->L+1 (86%), HOMO->L+2 (10%)
283.736167271	0.0255	HOMO->L+2 (13%), HOMO->L+3 (74%)
283.45075104	0.0369	HOMO->L+2 (39%), HOMO->L+3 (24%), HOMO->L+4 (28%)
280.380355071	0.0336	HOMO->L+2 (26%), HOMO->L+4 (53%)
273.726002897	0.0047	H-7->L+1 (14%), H-4->L+1 (72%)
270.619214258	0.0082	H-7->L+1 (41%), H-6->L+1 (16%), H-4->L+1 (16%)
267.709267403	0.0011	HOMO->L+7 (85%)
267.570608827	0.0162	H-10->LUMO (32%), H-5->L+1 (49%)
265.84941787	0.0632	H-10->LUMO (24%), H-7->L+1 (12%), HOMO->L+5 (35%)
264.719858682	0.0103	H-5->L+1 (22%), HOMO->L+5 (44%)
258.348842517	0.0119	H-8->L+1 (16%), H-7->L+1 (13%), H-6->L+1 (65%)
257.196600034	0.0066	H-8->L+1 (69%), H-7->L+1 (10%)
256.526096607	0.016	H-11->LUMO (77%)
256.40938291	0.0003	H-9->LUMO (10%), H-9->L+1 (84%)
251.01063492	0.1703	H-10->LUMO (15%), HOMO->L+6 (56%)
239.097855582	0.0086	H-12->LUMO (71%)
238.224984172	0.0345	H-12->LUMO (17%), H-2->L+2 (36%), H-1->L+5 (12%)

235.072318625	0.0118	H-3->L+3 (19%), H-1->L+3 (52%)
234.538700059	0.0607	H-1->L+2 (68%), H-1->L+3 (11%)
231.335372725	0.0329	H-1->L+4 (79%)
230.809972657	0.0001	H-13->LUMO (81%)
229.404938408	0.0001	H-2->L+7 (68%), HOMO->L+9 (21%)
227.803242958	0.0	H-2->L+7 (19%), H-1->L+7 (11%), HOMO->L+9 (57%)
227.235425777	0.0036	H-6->L+4 (10%), H-3->L+3 (33%), H-1->L+3 (29%)
225.548832112	0.0002	H-16->LUMO (35%), H-15->LUMO (59%)
221.990999288	0.0352	H-11->L+1 (19%), H-10->L+1 (50%)
220.181482884	0.0388	H-11->L+1 (14%), H-10->L+1 (30%), H-2->L+5 (11%), H-1->L+5 (13%)
219.150142311	0.0001	H-1->L+7 (74%)
218.562929491	0.0206	H-1->L+6 (20%), HOMO->L+8 (63%)
216.350869898	0.0128	H-11->L+1 (31%), H-2->L+2 (18%), H-2->L+4 (16%), H-1->L+5 (12%)
215.879985047	0.0016	H-2->L+3 (85%)
215.53097438	0.0104	H-11->L+1 (12%), H-2->L+4 (47%), H-1->L+5 (12%)
214.728425723	0.171	H-3->L+2 (25%), H-1->L+6 (23%)
213.28412209	0.0008	H-17->LUMO (57%), H-3->L+2 (15%)
212.804560455	0.0052	H-17->LUMO (12%), H-14->LUMO (30%), HOMO->L+10 (31%)
211.642130709	0.1265	H-3->L+4 (17%), H-2->L+5 (21%), H-1->L+5 (10%), H-1->L+6 (13%)
210.789358901	0.0006	H-18->LUMO (20%), H-16->LUMO (43%), H-15->LUMO (24%)
210.528073443	0.0953	H-14->LUMO (49%), H-3->L+2 (16%), HOMO->L+10 (10%)
209.929212686	0.0004	H-18->LUMO (71%), H-16->LUMO (11%)
209.037282527	0.0009	H-17->LUMO (12%), H-3->L+4 (25%)
207.327959419	0.0098	H-19->LUMO (89%)
206.286197049	0.0085	H-4->L+2 (29%), H-4->L+4 (40%)
206.135290226	0.0025	H-5->L+3 (14%), H-4->L+3 (71%)
205.08848548	0.1019	H-3->L+2 (15%), H-3->L+4 (18%), H-2->L+5 (20%), HOMO->L+10 (10%)
204.418968892	0.0112	H-2->L+6 (91%)
204.075769517	0.0001	H-9->L+2 (69%), H-9->L+4 (19%)
201.610148482	0.0046	H-12->L+1 (79%)
200.074542129	0.0202	H-5->L+3 (42%), H-3->L+3 (22%)
199.713588718	0.0645	H-4->L+2 (20%), H-3->L+5 (15%)
199.540022551	0.0013	H-13->L+1 (73%)
199.34431959	0.0061	H-3->L+5 (11%), H-3->L+6 (39%)
198.756320956	0.019	H-7->L+2 (11%), H-4->L+2 (15%), H-3->L+5 (35%)
198.447737587	0.0054	H-21->LUMO (11%), H-5->L+2 (30%), H-4->L+4 (14%), HOMO->L+11 (10%)
197.909226319	0.0068	H-7->L+2 (42%), H-6->L+2 (14%), H-4->L+2 (11%)
197.505683811	0.0001	H-5->L+7 (16%), H-4->L+7 (11%), H-3->L+7 (51%)
196.81905104	0.0115	H-8->L+3 (32%), H-7->L+3 (17%), H-6->L+3 (11%)
196.323520676	0.0017	H-21->LUMO (33%), H-8->L+3 (14%)

195.932604833	0.007	H-8->L+2 (10%), H-5->L+4 (21%)
195.355297344	0.0075	H-8->L+2 (11%), H-7->L+4 (14%), H-5->L+2 (12%), H-5->L+4 (25%)
195.201513024	0.0123	H-23->LUMO (42%), H-20->LUMO (24%)
194.604060542	0.0066	H-24->LUMO (13%), H-23->LUMO (22%), H-22->LUMO (11%), H-21->LUMO (10%), H-20->LUMO (31%)
193.904056884	0.0229	H-24->LUMO (16%), HOMO->L+11 (38%)
192.620742014	0.0019	H-24->LUMO (60%), H-23->LUMO (11%)
191.510956151	0.0249	H-8->L+2 (11%), H-8->L+4 (10%), H-7->L+4 (26%), H-6->L+2 (11%), H-6->L+4 (16%)
191.112436242	0.0175	H-7->L+2 (12%), H-7->L+4 (15%), H-6->L+2 (46%)
190.492875599	0.0014	H-8->L+3 (42%), H-7->L+3 (42%)
189.967506837	0.001	H-9->L+5 (87%)
189.906402518	0.0071	H-5->L+5 (17%), H-4->L+5 (32%), H-3->L+5 (20%)
189.854058667	0.0012	H-3->L+7 (15%), H-2->L+9 (11%), H-1->L+9 (57%)
189.008937927	0.0198	H-22->LUMO (36%), H-20->LUMO (11%), H-8->L+2 (16%)
188.936931231	0.0219	H-22->LUMO (28%), H-8->L+2 (24%), H-8->L+4 (15%)
188.520371938	0.0082	H-8->L+4 (12%), H-4->L+6 (42%)
187.883305065	0.0001	H-2->L+9 (77%)
187.428863208	0.0009	H-26->LUMO (49%)
187.301447258	0.0135	H-7->L+6 (13%), H-4->L+6 (20%), HOMO->L+12 (19%)
186.557415869	0.0471	H-5->L+6 (26%), H-1->L+8 (24%)
185.986518777	0.0003	H-5->L+7 (24%), H-4->L+7 (31%), H-3->L+7 (20%), H-1->L+9 (16%)
185.902857889	0.0534	H-14->L+1 (42%), H-4->L+5 (17%), H-1->L+10 (14%)
185.582853868	0.0223	H-5->L+5 (31%), H-4->L+5 (27%)
185.20030026	0.0108	H-16->L+1 (31%), H-15->L+1 (46%)
185.048272432	0.1062	H-5->L+6 (33%), H-1->L+8 (13%)
184.21519228	0.1433	H-6->L+4 (24%), H-6->L+6 (12%)
183.593249144	0.0197	H-16->L+1 (36%), H-15->L+1 (27%), H-7->L+7 (18%)
183.530742376	0.006	H-16->L+1 (14%), H-7->L+7 (54%), H-6->L+7 (14%)
183.178241874	0.0016	H-7->L+5 (67%), H-6->L+5 (22%)
182.773189375	0.3368	H-8->L+6 (13%), H-6->L+3 (16%)
182.490716827	0.1164	H-14->L+1 (13%), H-9->L+7 (19%), H-1->L+10 (24%)

Table S21. Major transitions calculated using TD-DFT studies of **8**.

Wavelength (nm)	**Osc. Strength**	**Major contribs**
646.761570225	1.3347	HOMO->LUMO (99%)
470.135723541	0.1898	H-1->LUMO (35%), HOMO->L+1 (64%)
415.454857126	0.0307	H-1->LUMO (60%), HOMO->L+1 (32%)
405.986420682	0.0005	H-2->LUMO (90%)

389.03104177	0.0503	H-3->LUMO (83%)
379.586054595	0.2291	H-5->LUMO (88%)
376.840196384	0.028	H-4->LUMO (95%)
365.239477441	0.0555	H-6->LUMO (89%)
352.037800654	0.1038	H-7->LUMO (89%)
349.931396269	0.3095	HOMO->L+2 (83%)
343.894247392	0.1428	H-1->L+1 (73%)
340.662709197	0.0179	H-9->LUMO (63%), H-8->LUMO (29%)
333.550867645	0.0386	H-10->LUMO (57%), H-9->LUMO (18%), H-8->LUMO (22%)
324.336707072	0.0027	H-2->L+1 (92%)
320.091374535	0.0632	H-10->LUMO (30%), H-9->LUMO (15%), H-8->LUMO (34%), H-1->L+1 (10%)
314.003274692	0.0502	H-3->L+1 (90%)
306.550112529	0.0265	H-11->LUMO (75%), H-4->L+1 (13%)
305.643271323	0.1357	H-11->LUMO (13%), H-4->L+1 (81%)
294.919583759	0.0078	H-5->L+1 (87%)
290.096148745	0.0049	HOMO->L+3 (96%)
288.960293221	0.0147	H-7->L+1 (56%), HOMO->L+4 (28%)
287.472913845	0.0151	H-7->L+1 (27%), HOMO->L+4 (61%)
284.687361972	0.0026	H-12->LUMO (84%)
282.154187366	0.0001	HOMO->L+5 (78%)
280.653265301	0.0036	H-6->L+1 (87%)
277.966534419	0.0096	HOMO->L+6 (66%)
274.519956187	0.1189	H-1->L+2 (86%)
267.917524931	0.0485	H-10->L+1 (16%), H-9->L+1 (27%), H-8->L+1 (43%)
265.155783939	0.0474	H-10->L+1 (40%), H-8->L+1 (28%), HOMO->L+7 (10%)
263.560633077	0.1095	HOMO->L+7 (48%), HOMO->L+8 (23%)
263.219313021	0.0692	H-8->L+1 (13%), H-2->L+2 (23%), HOMO->L+8 (42%)
261.752260038	0.0067	H-10->L+1 (25%), H-9->L+1 (60%)
260.871069102	0.0531	H-2->L+2 (32%), HOMO->L+7 (20%), HOMO->L+8 (17%)
259.066808083	0.0084	H-11->L+1 (72%)
257.629491973	0.0204	H-3->L+2 (47%)
253.702052409	0.0416	H-14->LUMO (45%), H-13->LUMO (32%), HOMO->L+9 (11%)
252.80195949	0.0523	H-14->LUMO (33%), H-13->LUMO (46%)
247.251357089	0.0043	H-15->LUMO (86%)
246.646361527	0.1574	H-4->L+2 (47%), HOMO->L+9 (28%)
244.621957644	0.0017	H-12->L+1 (74%)
243.804210116	0.0063	H-12->L+1 (11%), H-4->L+2 (21%), HOMO->L+9 (28%), HOMO->L+10 (14%)
239.865721937	0.0058	H-1->L+3 (84%)
239.559835788	0.0422	HOMO->L+9 (11%), HOMO->L+10 (68%)
238.224984172	0.0159	H-1->L+4 (92%)

237.344831372	0.0015	H-5->L+2 (78%)
236.5839656	0.0085	H-17->LUMO (53%), H-16->LUMO (34%)
232.860403073	0.0178	H-17->LUMO (34%), H-16->LUMO (35%), H-11->L+2 (13%)
232.167093632	0.0059	H-16->LUMO (13%), H-11->L+2 (49%), H-1->L+5 (12%)
230.304064293	0.0235	H-11->L+2 (17%), H-7->L+2 (45%), H-1->L+5 (19%)
229.54084684	0.0057	H-11->L+2 (11%), H-7->L+2 (37%), H-1->L+5 (29%)
229.345529064	0.0045	H-9->L+4 (15%), H-5->L+3 (46%)
228.012713352	0.0207	H-1->L+5 (12%), H-1->L+6 (15%), HOMO->L+11 (36%)
225.454499686	0.0293	H-1->L+6 (32%), HOMO->L+11 (35%)
224.743402781	0.0126	H-6->L+2 (61%), H-1->L+6 (13%)
222.989142304	0.0015	H-3->L+8 (37%), H-2->L+8 (34%)
222.026777358	0.087	H-14->L+1 (12%), H-2->L+5 (10%), H-1->L+7 (47%)
221.744841114	0.063	H-8->L+2 (22%), H-6->L+2 (22%)
220.056428618	0.0038	H-14->L+1 (29%), H-13->L+1 (11%), H-1->L+7 (14%), HOMO->L+12 (18%)
219.316834735	0.0811	H-14->L+1 (12%), H-13->L+1 (34%), H-1->L+7 (10%), HOMO->L+12 (24%)
218.401227804	0.0233	H-14->L+1 (16%), H-4->L+5 (10%), H-2->L+4 (14%), H-2->L+5 (13%)
217.676521318	0.0005	H-3->L+3 (13%), H-2->L+3 (81%)
217.420768106	0.1291	H-15->L+1 (10%), H-8->L+2 (15%), H-2->L+6 (14%)
216.869324842	0.0053	H-13->L+1 (17%), H-2->L+4 (22%), HOMO->L+12 (17%)
216.471746857	0.0046	H-13->L+1 (14%), H-2->L+4 (13%), H-1->L+8 (25%), HOMO->L+12 (11%)
215.842402793	0.0388	H-2->L+4 (23%), H-1->L+8 (20%)
215.504750421	0.0091	H-20->LUMO (90%)
215.123352556	0.011	H-15->L+1 (46%)
214.279381643	0.002	H-10->L+2 (52%), H-9->L+2 (27%)
213.717947722	0.0065	H-4->L+5 (13%), H-2->L+5 (22%), H-2->L+6 (15%)
212.88860216	0.0733	H-15->L+1 (14%), H-9->L+2 (12%), H-3->L+4 (12%), H-2->L+6 (13%)
212.614797497	0.0316	H-10->L+2 (29%), H-9->L+2 (34%), H-8->L+2 (11%)
212.007648659	0.0041	H-3->L+3 (72%), H-2->L+3 (12%)
211.7252566	0.1001	H-5->L+4 (17%), H-3->L+5 (31%)
211.620456428	0.0284	H-18->LUMO (54%)
211.382332002	0.0001	H-22->LUMO (11%), H-18->LUMO (15%), H-3->L+5 (10%)
210.710547088	0.0104	H-3->L+4 (22%), H-3->L+5 (20%), H-3->L+6 (23%)
210.124892826	0.0734	H-22->LUMO (22%), H-3->L+4 (18%), H-3->L+6 (14%), H-2->L+7 (10%)
209.900780477	0.0082	H-23->LUMO (72%)
209.270149904	0.0015	H-12->L+2 (77%)
209.07605776	0.0159	H-6->L+3 (85%)
208.671389882	0.0046	H-19->LUMO (31%), H-6->L+4 (15%)
208.587134947	0.0141	H-22->LUMO (12%), H-19->LUMO (12%), H-6->L+4 (45%)
208.488923475	0.0003	H-4->L+3 (90%)
208.345280566	0.0063	H-19->LUMO (25%), H-2->L+9 (12%), H-2->L+10 (17%)

207.887647572	0.0104	H-6->L+4 (21%), H-5->L+4 (17%), H-4->L+4 (29%)
207.508398487	0.0077	H-4->L+4 (57%)
206.046221748	0.0172	H-3->L+7 (15%), H-2->L+7 (26%), H-2->L+10 (12%)
204.959652536	0.0239	H-16->L+1 (18%), H-5->L+5 (14%), H-1->L+9 (34%)
204.462792942	0.0284	H-21->LUMO (61%)
203.837555302	0.0058	H-16->L+1 (15%), H-5->L+5 (48%)
203.737068461	0.0036	H-24->LUMO (62%)
203.519686494	0.0148	H-24->LUMO (22%), H-4->L+8 (20%)
203.169509238	0.0043	H-16->L+1 (12%), H-4->L+8 (13%), H-1->L+9 (16%), HOMO->L+13 (11%)
202.333980143	0.1483	H-4->L+6 (12%), H-3->L+7 (38%)
201.12611406	0.0072	H-10->L+3 (12%), H-7->L+3 (56%), H-5->L+3 (10%)
200.73210668	0.0168	H-7->L+4 (31%), H-1->L+10 (13%), HOMO->L+13 (13%)
200.459487489	0.0023	H-5->L+6 (39%), H-4->L+7 (26%)
200.006764014	0.0185	H-25->LUMO (18%), H-5->L+7 (34%)
199.723240137	0.0199	H-7->L+4 (18%), H-5->L+6 (19%), H-4->L+7 (22%)
199.681424059	0.0006	H-25->LUMO (43%), H-1->L+10 (26%)

Table S22. Major transitions calculated using TD-DFT studies of **8-Re(I)**.

Wavelength (nm)	**Osc. Strength**	**Major contribs**
636.109963636	0.7275	HOMO->LUMO (97%)
599.913838546	0.0104	H-1->LUMO (98%)
567.615222324	0.0004	H-2->LUMO (99%)
492.998500983	0.0143	H-3->LUMO (40%), HOMO->L+1 (57%)
471.279432158	0.0382	H-4->LUMO (64%), H-3->LUMO (25%)
446.130736613	0.0016	H-1->L+1 (98%)
427.811990657	0.0068	H-2->L+1 (97%)
424.21115069	0.0802	H-6->LUMO (22%), H-5->LUMO (70%)
421.242119431	0.2827	H-6->LUMO (27%), H-5->LUMO (11%), H-4->LUMO (18%), H-3->LUMO (17%), HOMO->L+1 (11%)
412.922776967	0.0934	H-7->LUMO (14%), H-6->LUMO (49%), H-5->LUMO (10%)
403.410532349	0.0863	H-7->LUMO (69%)
401.06163231	0.0338	H-8->LUMO (96%)
391.376599679	0.0535	H-10->LUMO (21%), H-9->LUMO (69%)
381.138004956	0.1121	H-10->LUMO (47%), HOMO->L+2 (44%)

377.4827006	0.1235	H-10->LUMO (27%), HOMO->L+2 (46%)
373.176598279	0.0457	H-4->L+1 (20%), H-3->L+1 (71%)
361.83917412	0.013	H-12->LUMO (16%), H-11->LUMO (11%), H-4->L+1 (58%), H-3->L+1 (10%)
359.145452211	0.028	H-11->LUMO (84%), H-4->L+1 (10%)
352.618506334	0.0109	H-13->LUMO (72%), H-12->LUMO (20%)
347.94766933	0.0059	H-14->LUMO (86%)
346.993347548	0.0573	H-1->L+2 (83%)
344.46751594	0.0218	H-13->LUMO (12%), H-12->LUMO (29%), HOMO->L+3 (34%)
342.829235482	0.0019	H-15->LUMO (97%)
338.986173649	0.0013	H-5->L+1 (14%), H-2->L+2 (74%)
337.757962875	0.0095	H-6->L+1 (15%), H-5->L+1 (56%), H-2->L+2 (23%)
334.29732801	0.048	H-6->L+1 (72%), H-5->L+1 (18%)
327.818389287	0.1396	H-7->L+1 (78%), HOMO->L+3 (12%)
324.328222801	0.0726	H-8->L+1 (11%), H-7->L+1 (15%), HOMO->L+3 (31%)
322.539523965	0.0866	H-8->L+1 (83%)
318.668088036	0.0024	H-1->L+3 (13%), HOMO->L+4 (80%)
314.808533953	0.0071	H-9->L+1 (88%)
314.281858079	0.0065	H-1->L+3 (69%), HOMO->L+4 (15%)
306.679017048	0.0049	H-10->L+1 (94%)
305.424922432	0.0097	H-3->L+2 (10%), H-2->L+3 (37%), H-1->L+4 (42%)
303.994588727	0.0019	H-3->L+2 (72%)
298.973216813	0.0033	H-2->L+4 (84%)
298.003107829	0.0096	H-11->L+1 (90%)
296.18775206	0.0526	H-2->L+3 (31%), H-1->L+4 (28%), HOMO->L+5 (19%)
294.653246381	0.0427	H-12->L+1 (23%), H-4->L+2 (11%), HOMO->L+5 (36%)
293.766598773	0.0984	H-13->L+1 (20%), H-4->L+2 (61%)
292.574257291	0.0077	H-13->L+1 (48%), HOMO->L+5 (14%)
291.67260989	0.0011	H-16->LUMO (94%)
290.164040844	0.039	H-14->L+1 (63%), HOMO->L+6 (15%)
289.919777884	0.0136	H-14->L+1 (23%), HOMO->L+6 (67%)
288.254889362	0.0117	H-13->L+1 (15%), H-12->L+1 (40%), HOMO->L+7 (24%)
286.569266179	0.0032	H-15->L+1 (97%)
284.654681358	0.0528	H-12->L+1 (11%), HOMO->L+7 (65%)
283.924596987	0.0101	H-1->L+5 (77%)
283.645290687	0.0095	HOMO->L+9 (98%)
283.056008886	0.0036	HOMO->L+8 (82%)
280.984006827	0.0066	H-4->L+3 (21%), H-3->L+3 (61%)
274.933903256	0.0048	H-17->LUMO (13%), H-6->L+2 (23%), H-5->L+2 (26%), HOMO->L+10 (21%)
274.386298881	0.0331	H-17->LUMO (34%), H-6->L+2 (12%), H-5->L+2 (17%), HOMO->L+10 (19%)
272.91259743	0.005	H-7->L+2 (10%), H-6->L+2 (33%), H-5->L+2 (34%)

272.211546342	0.0137	H-2->L+5 (62%)
270.023941572	0.0433	H-17->LUMO (16%), HOMO->L+10 (26%), HOMO->L+11 (27%)
268.683915944	0.031	H-7->L+2 (53%), H-5->L+2 (14%)
268.29436729	0.0302	H-1->L+6 (86%)
267.074926248	0.0154	H-8->L+2 (10%), H-4->L+3 (51%), H-3->L+3 (17%), HOMO->L+11 (12%)
262.917897687	0.0155	H-1->L+8 (66%)
262.394855161	0.0054	H-2->L+6 (81%)
262.001168615	0.0197	H-3->L+4 (36%), HOMO->L+12 (19%)
261.509339631	0.0314	H-3->L+4 (15%), HOMO->L+12 (63%)
258.888294277	0.0104	H-18->LUMO (58%), H-8->L+2 (10%), H-2->L+8 (11%)
258.618287087	0.001	H-9->L+2 (87%)
258.031619172	0.0038	H-1->L+7 (70%), H-1->L+10 (15%)
257.854528653	0.0356	H-18->LUMO (11%), H-2->L+8 (70%)
256.988689009	0.0116	H-18->LUMO (13%), H-8->L+2 (24%), H-3->L+5 (10%)
256.218625774	0.1673	H-3->L+5 (10%), HOMO->L+10 (10%), HOMO->L+11 (34%)
255.605890018	0.0021	H-4->L+4 (69%), H-3->L+4 (12%)
254.446596368	0.0344	H-5->L+3 (11%), H-3->L+5 (12%), H-1->L+10 (20%), H-1->L+11 (14%)
254.045145915	0.0032	H-1->L+9 (84%)
253.644960234	0.0086	H-1->L+9 (13%), H-1->L+10 (23%), H-1->L+11 (12%)
253.065117491	0.0008	H-19->LUMO (55%), H-6->L+3 (15%)
252.092621309	0.0025	H-19->LUMO (23%), H-6->L+3 (32%), H-5->L+3 (17%)
251.637257235	0.0016	H-2->L+7 (81%)
251.21916198	0.0012	H-10->L+2 (91%)
249.852272157	0.004	H-16->L+1 (14%), H-7->L+3 (24%), H-6->L+3 (19%), H-5->L+3 (21%)
249.686227268	0.005	H-16->L+1 (83%)
248.989241916	0.001	HOMO->L+13 (88%)
248.619769821	0.0046	H-13->L+2 (24%), H-11->L+2 (45%)
248.087468009	0.0002	H-2->L+9 (95%)
247.918802264	0.0017	H-1->L+10 (29%), H-1->L+11 (56%)
247.438866849	0.001	H-14->L+2 (21%), H-13->L+2 (10%), H-11->L+2 (33%)
247.049362396	0.0106	H-13->L+2 (11%), H-12->L+2 (13%), H-7->L+3 (27%), H-5->L+3 (12%)
246.670897106	0.0075	H-2->L+10 (44%), H-2->L+11 (11%)
245.98086067	0.0139	H-8->L+3 (49%)
245.508391937	0.0038	HOMO->L+14 (76%)
244.53993612	0.0022	H-15->L+2 (58%), H-14->L+2 (13%)
243.866550643	0.0017	H-4->L+5 (41%), H-3->L+5 (11%)
243.449954862	0.0013	H-6->L+4 (48%), H-5->L+4 (18%), H-3->L+6 (11%)
243.053837432	0.004	H-20->LUMO (54%), H-17->L+1 (13%)
242.687505896	0.0064	H-15->L+2 (18%), H-12->L+2 (31%)
242.246523148	0.003	H-1->L+12 (73%)

241.726995013	0.0032	H-3->L+6 (44%), H-2->L+11 (15%)
241.477471588	0.0013	H-14->L+2 (38%), H-13->L+2 (33%)
241.32706519	0.006	H-3->L+6 (18%), H-2->L+11 (38%)
240.891008203	0.0113	H-7->L+4 (30%), H-6->L+4 (10%), H-5->L+4 (18%)
239.125524142	0.0012	H-23->LUMO (13%), H-22->LUMO (73%)
238.899751459	0.0033	H-3->L+8 (60%)
238.316565136	0.0011	H-8->L+4 (25%), H-7->L+4 (32%)
237.936963637	0.0584	HOMO->L+15 (41%)
237.658749472	0.022	H-8->L+4 (12%), H-5->L+4 (23%), H-2->L+12 (20%), H-2->L+13 (16%)
237.163229298	0.0024	H-9->L+3 (73%)
236.742076745	0.0024	H-17->L+1 (21%), H-9->L+3 (16%), H-3->L+7 (28%)
236.543342578	0.0204	H-8->L+4 (24%), H-2->L+12 (34%)
235.908731662	0.0009	H-2->L+12 (21%), H-2->L+13 (55%)
235.532281558	0.0013	H-21->LUMO (22%), H-3->L+9 (35%)
235.290911702	0.0028	H-21->LUMO (24%), H-3->L+7 (36%), H-3->L+9 (15%)
235.161491213	0.0189	H-4->L+6 (68%)
234.916429217	0.0121	H-8->L+4 (16%), H-1->L+13 (37%), H-1->L+14 (20%)
233.645892796	0.0136	H-21->LUMO (36%), H-17->L+1 (11%)
233.241516662	0.0034	H-6->L+5 (44%), H-5->L+5 (15%), H-4->L+8 (23%)
231.503833394	0.0005	H-23->LUMO (31%), H-10->L+3 (45%)
231.400136268	0.0002	H-23->LUMO (25%), H-10->L+3 (20%), H-4->L+7 (15%)
231.037926752	0.0032	H-23->LUMO (17%), H-10->L+3 (10%), H-4->L+7 (36%)
230.883040991	0.0038	H-7->L+5 (11%), H-5->L+5 (30%), H-4->L+8 (27%)
230.214262129	0.0175	H-4->L+7 (15%), H-3->L+10 (12%), H-1->L+14 (35%)
229.557846718	0.0038	H-4->L+9 (14%), H-1->L+15 (18%)
229.464378539	0.004	H-3->L+10 (22%), H-1->L+15 (13%)
229.392205244	0.0004	H-1->L+14 (10%), H-1->L+15 (12%)
229.209851757	0.0292	H-14->L+3 (16%), H-13->L+3 (24%), H-6->L+5 (10%)
228.960117103	0.0076	H-6->L+5 (12%), H-1->L+15 (30%)
228.786892922	0.0011	H-25->LUMO (35%), H-24->LUMO (33%), H-4->L+9 (15%)
227.895362496	0.0004	H-9->L+4 (90%)
227.723745086	0.0129	H-2->L+14 (47%), HOMO->L+16 (13%)
227.556562379	0.0139	H-11->L+3 (11%), H-4->L+10 (10%), H-2->L+14 (25%), HOMO->L+16 (16%)
226.774080464	0.0027	H-11->L+3 (68%), HOMO->L+16 (18%)
226.711880142	0.0031	H-4->L+10 (27%), HOMO->L+16 (24%)
226.401389647	0.0058	H-7->L+5 (20%), H-5->L+9 (12%), H-4->L+9 (15%), HOMO->L+16 (17%)
226.153608909	0.0024	H-15->L+3 (26%), H-3->L+11 (10%)
225.922835715	0.0023	H-8->L+5 (48%)
225.713076665	0.003	H-25->LUMO (18%), H-24->LUMO (20%)
225.548832112	0.0099	H-25->LUMO (19%), H-24->LUMO (18%), H-7->L+5 (10%)

224.992184176	0.0051	H-12->L+3 (11%), H-4->L+10 (11%), H-3->L+11 (14%), H-2->L+15 (20%)
224.633461993	0.011	H-12->L+3 (50%), H-2->L+15 (15%)
224.032729233	0.0032	H-4->L+12 (16%), H-3->L+12 (31%), H-2->L+15 (10%)
223.620577542	0.019	H-18->L+1 (55%), H-8->L+5 (10%)
223.125583552	0.0027	H-14->L+3 (22%), H-13->L+3 (13%), H-3->L+11 (11%), H-2->L+15 (11%)
222.949044276	0.0056	H-27->LUMO (12%), H-26->LUMO (62%)
222.508915871	0.0039	H-14->L+4 (15%), H-13->L+4 (21%), H-10->L+4 (29%)
222.433069631	0.0128	H-1->L+16 (15%), HOMO->L+18 (29%)
222.273562231	0.0014	H-10->L+4 (59%)
222.030753411	0.0027	H-6->L+6 (13%), H-6->L+8 (10%), H-5->L+6 (52%)
221.92344994	0.0045	H-1->L+16 (29%), HOMO->L+18 (17%)
221.855941688	0.0058	H-28->LUMO (27%), H-27->LUMO (43%), H-26->LUMO (14%)
221.459664218	0.0426	H-14->L+3 (10%), H-13->L+3 (13%)
221.080567415	0.0346	H-15->L+3 (11%), HOMO->L+18 (11%)
220.915120382	0.0066	H-6->L+10 (11%), H-4->L+11 (10%)
220.608517664	0.0046	H-6->L+6 (25%)

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S2. S. Uchiyama, Y. Matsumura, A. P. de Silva and K. Iwai, *Anal. Chem*., **2003**, 75, 5926.

S3. J. R. Lakowicz, Principles of Fluorescence Spectroscopy, 3rd edn., Springer Science, 2006, pp. 141-143.

S4. Given in reference no.32 in the main paper.

S5. Given in reference no. 33 in the main paper.

S6. Given in reference no. 34 in the main paper.

S7. Given in reference no. 35 in the main paper.