Supplementary Information (SI) for Organic & Biomolecular Chemistry.
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Synthesis and Studies of *Meso*-Phenothiazinyl 3-Pyrrolyl BODIPY and Its Derivatives

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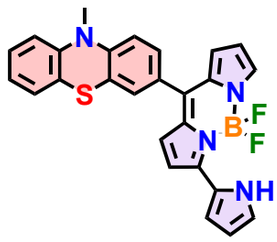
Supporting Information

Experimental Section

- All chemicals including Boron trifluoride etherate ($BF_3{\cdot}OEt_2$), 2, 3-dichloro-5, 6-dicyano-1, 4-benzoquinone (DDQ) were procured from Aldrich and used as received. Neutral alumina and silica gel (60-120 mesh) column chromatographic methods were used for purification purposes. Reported methods were used for the synthesis of compounds**,** **7** and **8**.[1-2] The ^{1}H & ^{13}C NMR spectra were recorded in $CDCl_3$ on Bruker 400 and 500 MHz instruments. The ^{13}C NMR frequencies are 125.77 and 100.06 MHz for 500 MHz and 400 MHz instruments respectively.
- Agilent UV-Visible-NIR Spectrophotometer was used for carrying out absorption spectral studies and steady-state fluorescence spectra were obtained with PerkinElmer Lambda-35. The exponential decay curve of compounds was fitted appropriately with a biexponential equation. The average lifetime (τ_{av}) was calculated following the equations depicted in the literature.
- Fluorescence quantum yields were determined in solution by comparing the corrected spectrum with that of Rhodamine 6G (Φ =0.95) in toluene by taking the area under total emission using the procedure reported earlier.[3]
- Bruker maXis Impact, Q-TOF, and MALDI -TOF mass spectrometer instruments were used for recording HR mass spectra.
- **Computational information:** All computations were performed using the Gaussian 09 program package, unless otherwise mentioned. The density functional theory (DFT)[4] method, with hybrid functional B3LYP [5] in conjunction with basis set 6-31G(d,p)[6] was implemented to optimize the structure of macrocycles **4a** in the ground (S_0) states. To increase the accuracy of electronic structure calculations and the geometry optimization in the S_0 state, dispersive interactions in the electron density of the macrocycle were studied using Grimme's D3 dispersion correction method (GD3BJ) over the B3LYP functional. Oscillator strengths were obtained using identical basis and functional hybrid set B3LYP /6-31G whereas the vertical excitation energies were obtained by the help of TD-DFT techniques for $S_0 \rightarrow$ Sn transitions.[7] Under the Polarizable Continuum Model (PCM)[8] in the toluene media, all the computations were done using the Self-Consistent Reaction Field (SCRF). The electronic absorption spectra and oscillator strengths were thoroughly examined using Time-dependent (TD)-DFT with the PCM model based on the optimized structures in the S_0 state.

- **^{1}H, ^{13}C, and Mass spectra:**



Compound 3

Compound Details

Cpd. 1: C26 H19 B F2 N4 S

Formula	m/z	Observed M/Z	Difference_Da	Difference_PPM	Score
C26 H19 B F2 N4 S	469.1463	469.146331888221	-0.761577997593577	-1.63028954023604	93.01

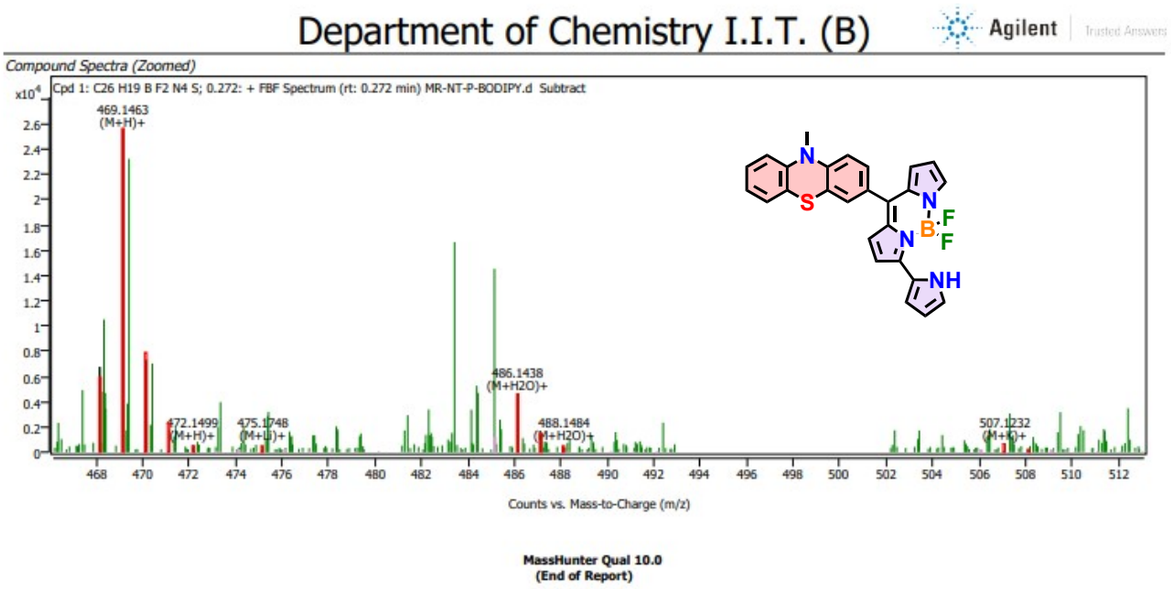


Figure S1. HR mass spectrum of compound **3.**

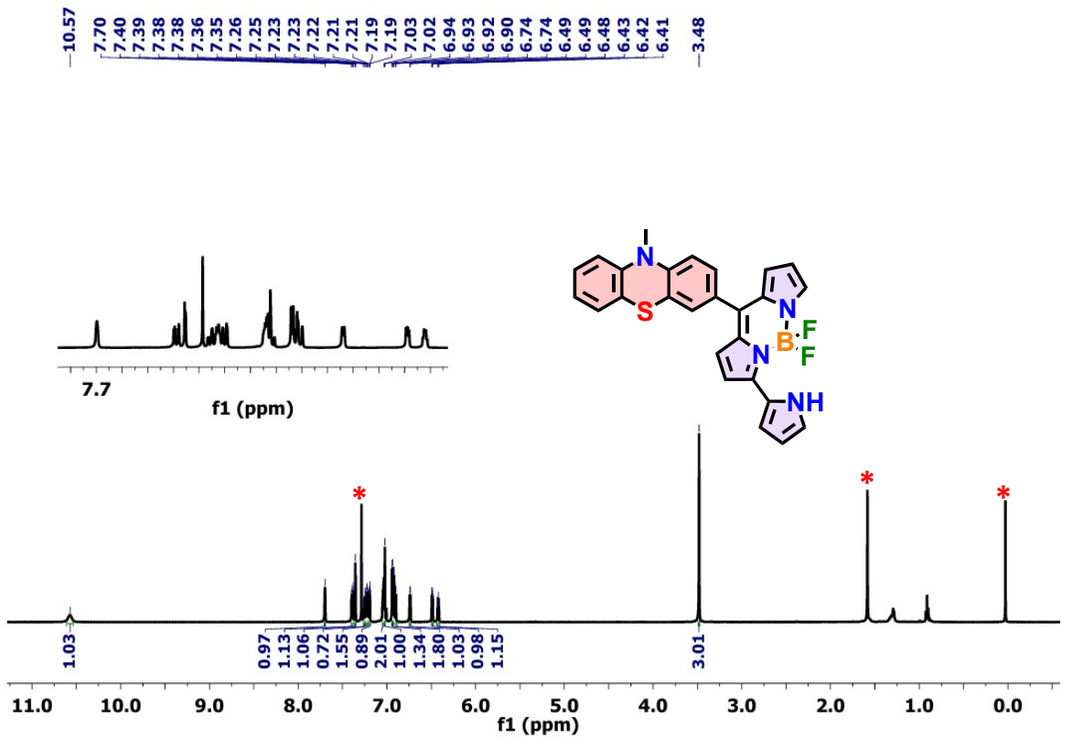


Figure S2. ^{1}H NMR spectrum of the compound **3** recorded in $CDCl_3$ on 400 MHz NMR instrument. The expansion of the aromatic region is shown in the inset. Note: Peaks marked with an asterisk (*) are due to residual solvents.

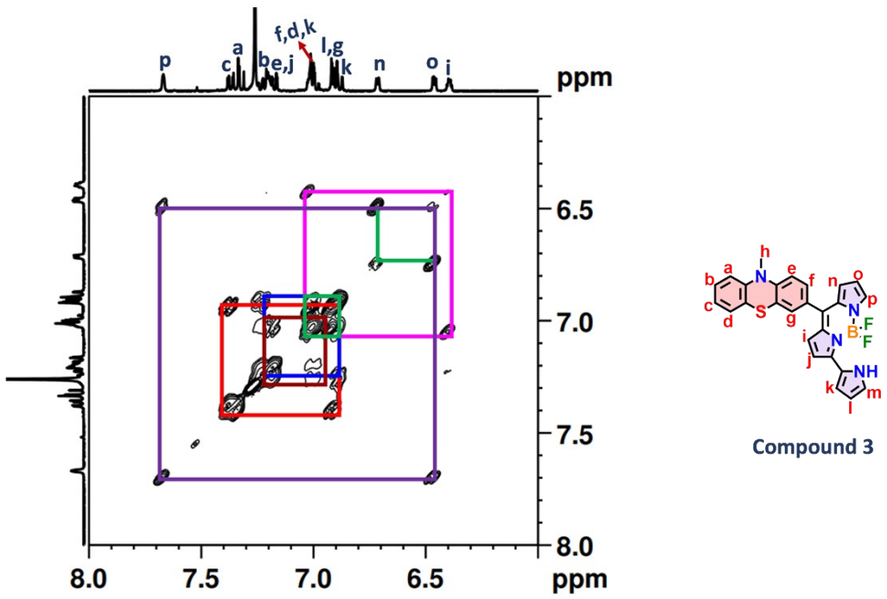


Figure S3. ^{1}H-^{1}H COSY spectrum of compound **3** recorded in $CDCl_3$ at 25 °C.

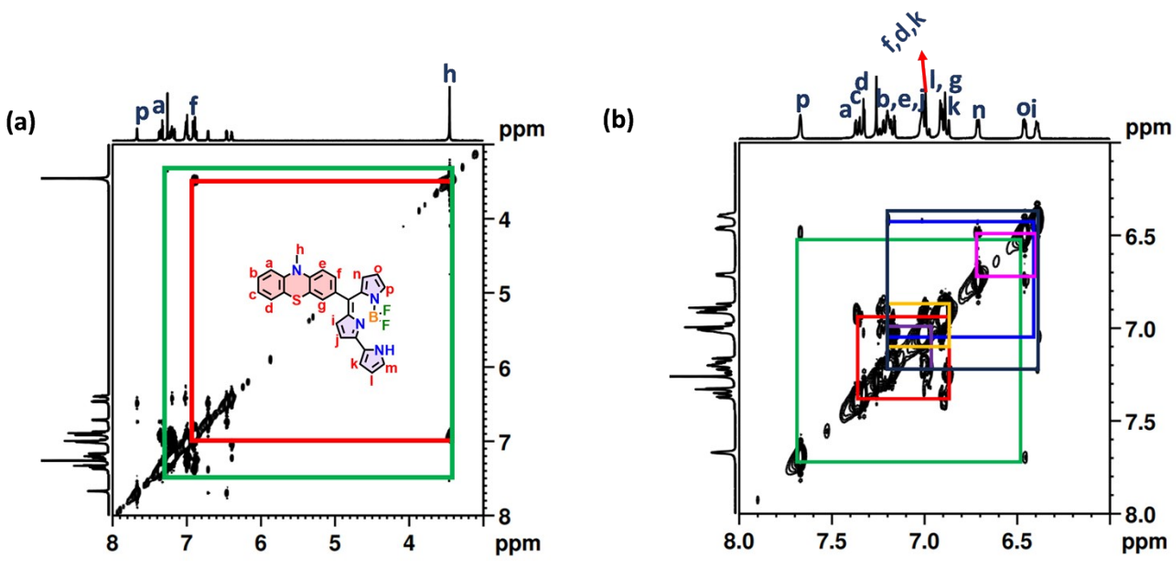


Figure S4. ^{1}H-^{1}H NOESY **(a)** expanded, **(b)** full spectrum of compound **3** recorded in $CDCl_3$ at 25 °C.

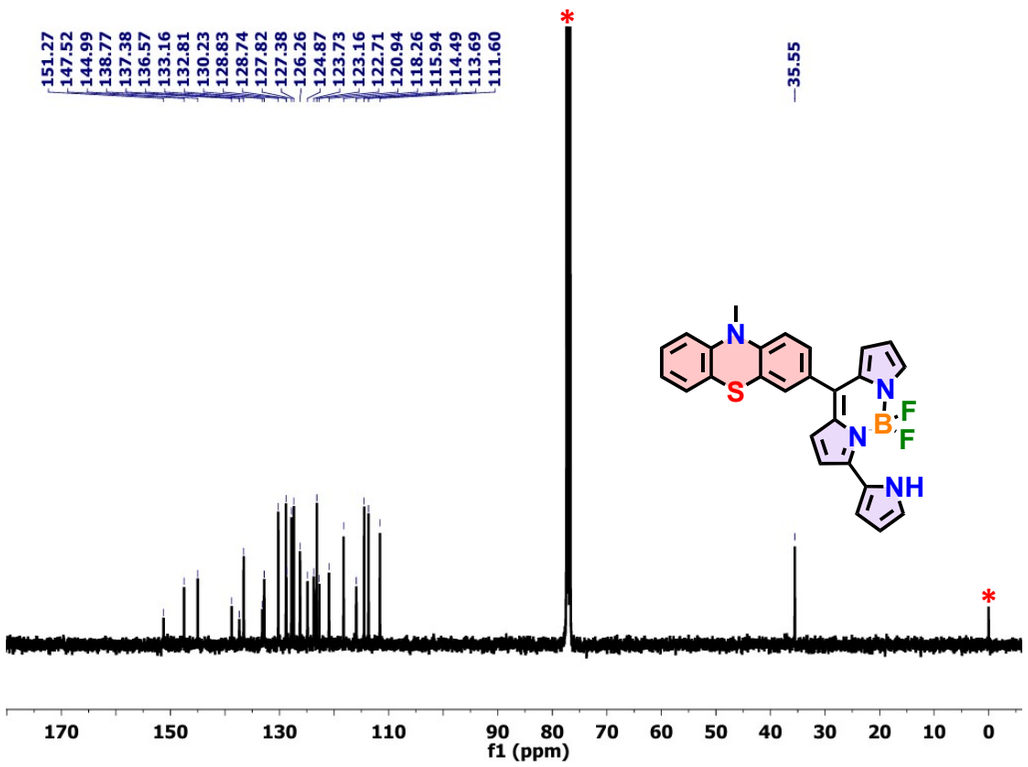


Figure S5. $^{13}C\{1H\}$ NMR spectrum of the compound **3** recorded in $CDCl_3$ on 100.06 MHz NMR instrument; Note: Peaks marked with an asterisk (*) are due to residual solvents.

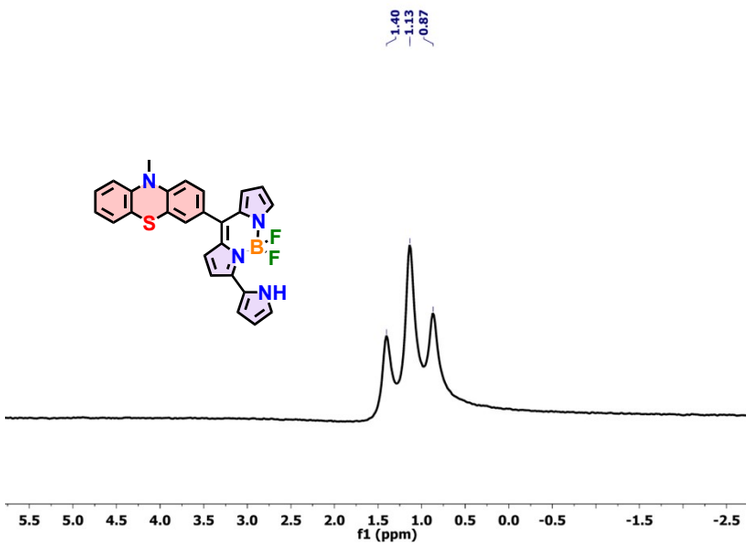


Figure S6. ^{11}B NMR spectrum of the compound **3** recorded in $CDCl_3$.

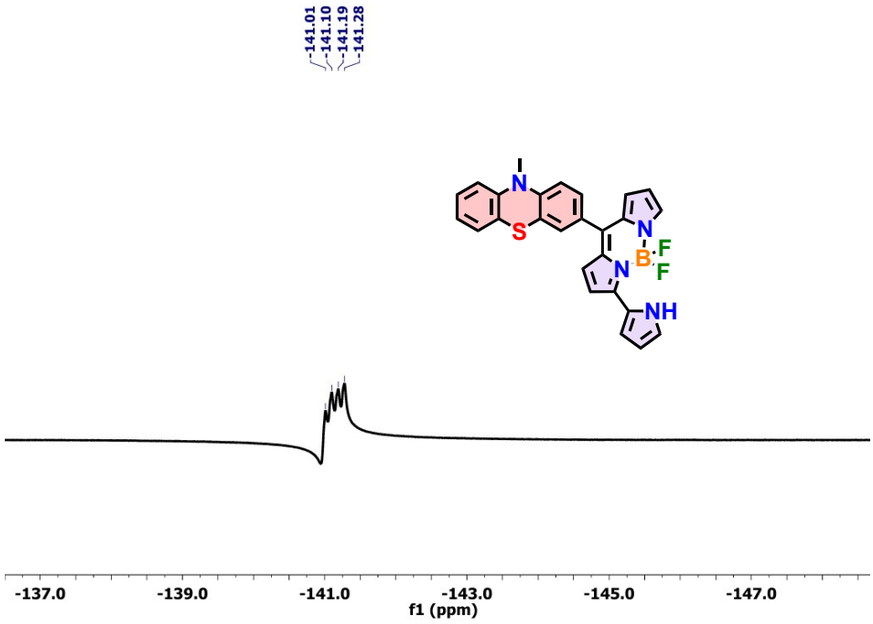
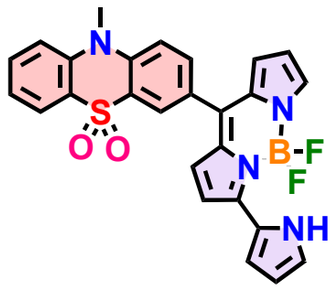


Figure S7. ^{19}F NMR spectrum of the compound **3** recorded in $CDCl_3$



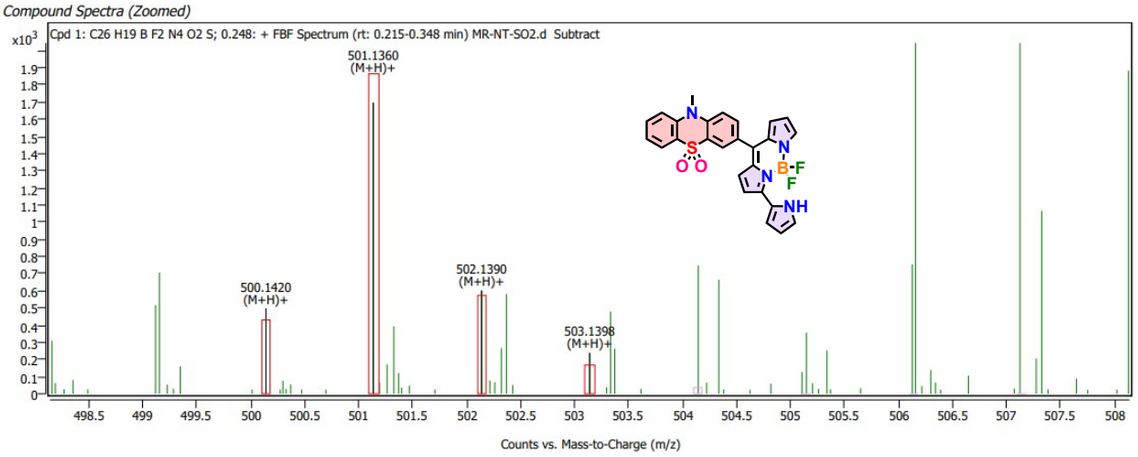
Compound 3.SO_2

Compound Details

Cpd. 1: C26 H19 B F2 N4 O2 S

Formula	m/z	Observed M/Z	Difference_Da	Difference_PPM	Score
C26 H19 B F2 N4 O2 S	501.1360	501.135978893616	0.045405465471049	0.0909687407644461	87.02

Compound Spectra (Zoomed)



MassHunter Qual 10.0
(End of Report)

Figure S8. HR mass spectrum of compound **3.SO_2**.

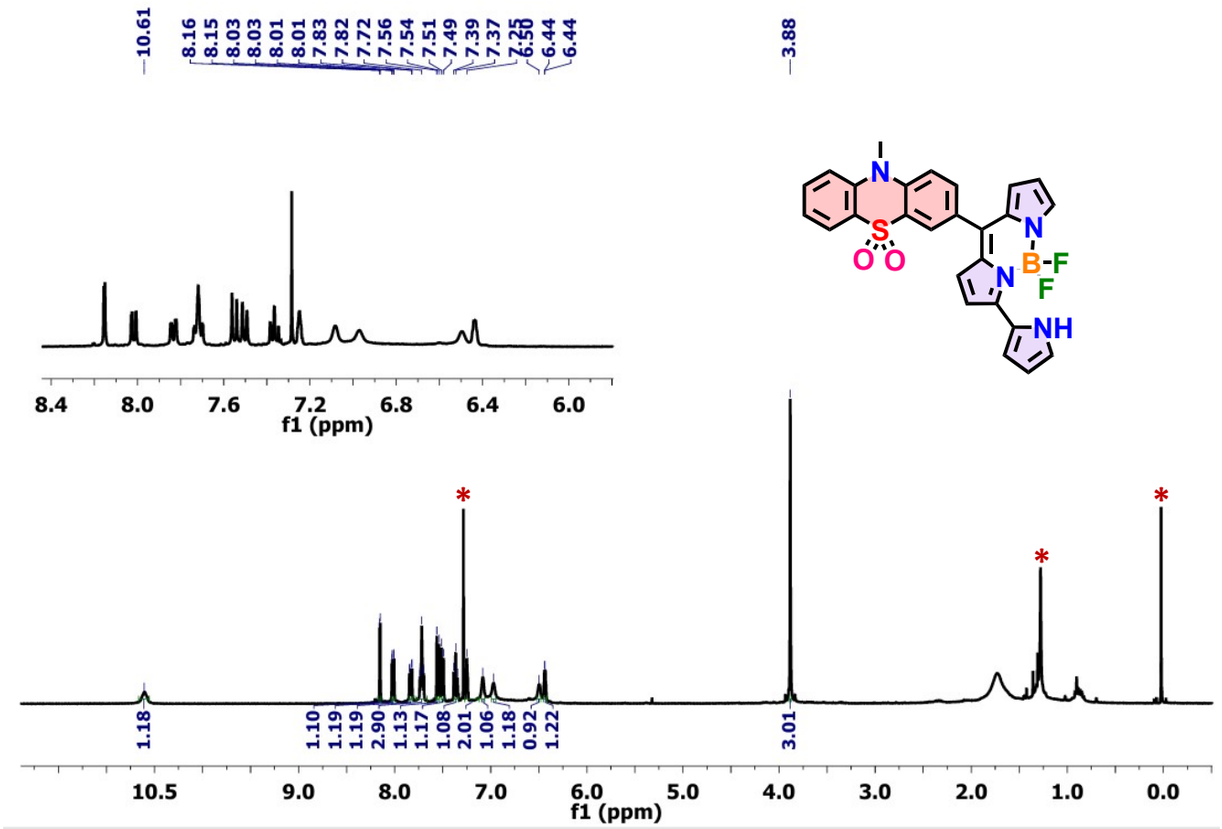


Figure S9. ^{1}H NMR spectrum of the compound **3.SO$_2$** recorded in $CDCl_3$ on 400 MHz NMR instrument. The expansion of the aromatic region is shown in the inset. Note: Peaks marked with an asterisk (*) are due to residual solvents.

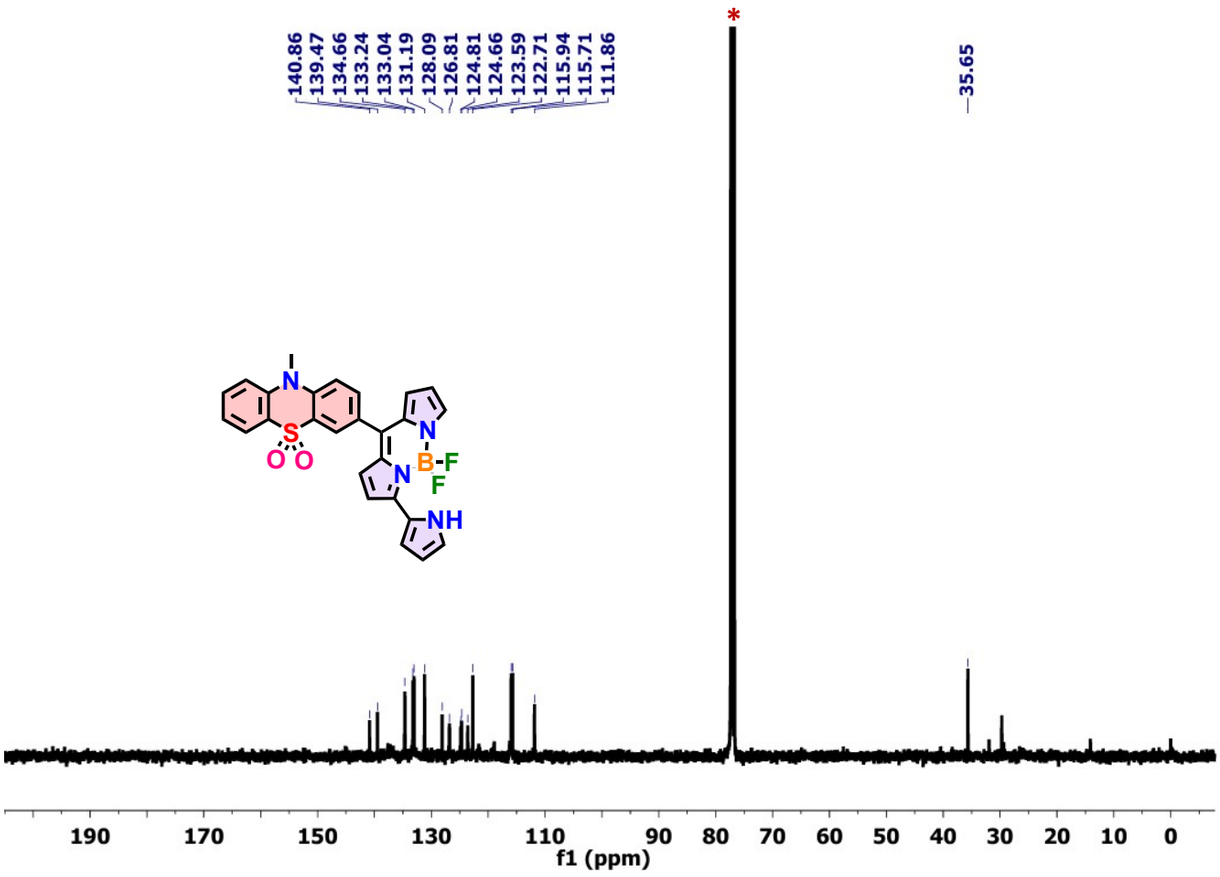


Figure S10. $^{13}C\{1H\}$ NMR spectrum of the compound **3.SO$_2$** recorded in $CDCl_3$ on 100.06 MHz NMR instrument; Note: Peaks marked with an asterisk (*) are due to residual solvents.

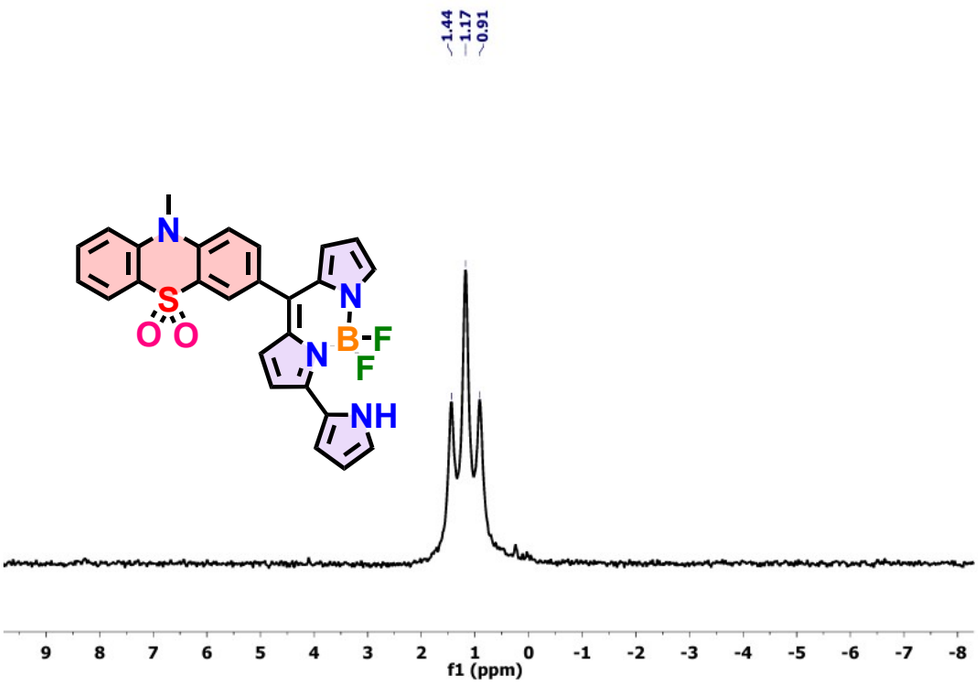


Figure S11. ^{11}B NMR spectrum of the compound **3.SO$_2$** recorded in $CDCl_3$.

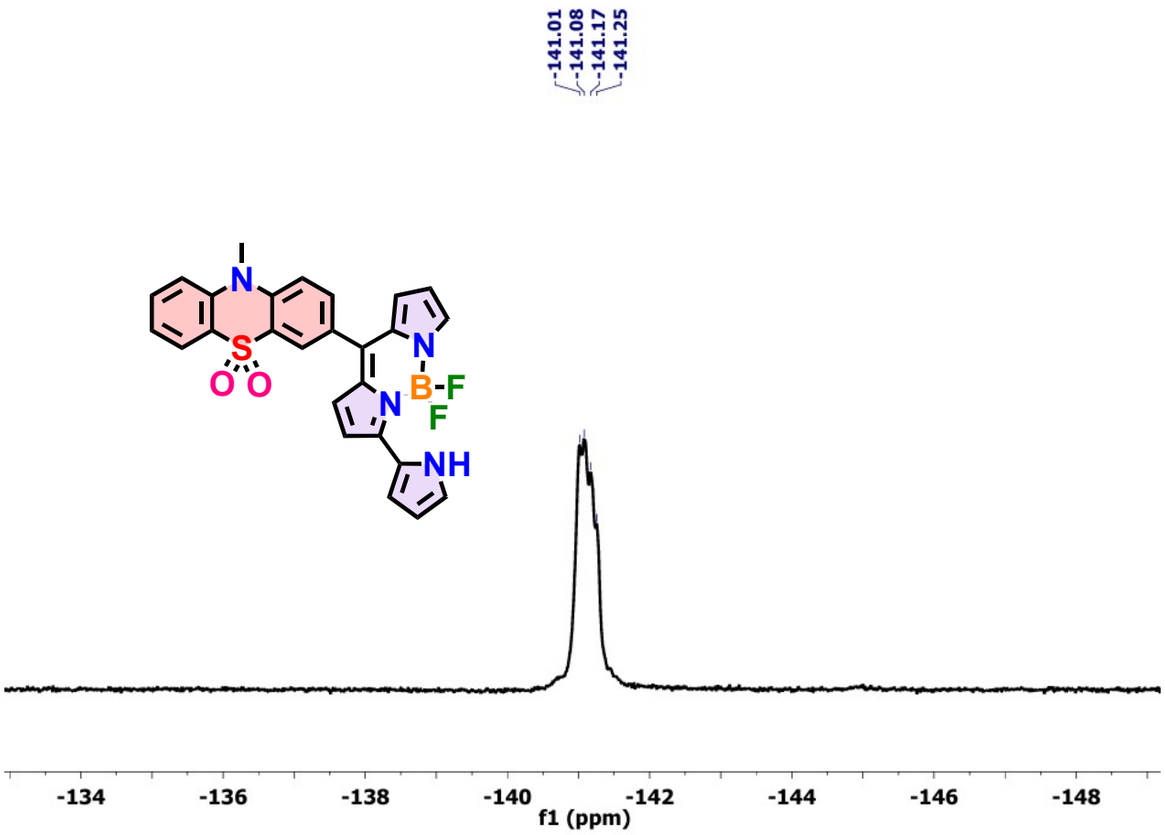
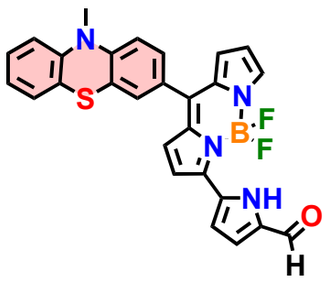


Figure S12. ^{19}F NMR spectrum of the compound **3.SO$_2$** recorded in $CDCl_3$



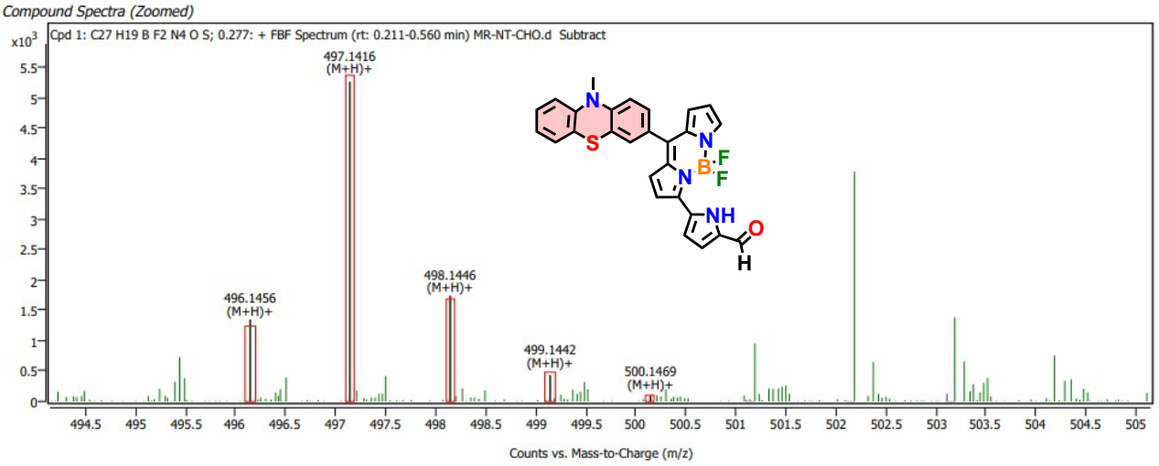
Compound 4

Compound Details

Cpd. 1: C27 H19 B F2 N4 O S

Formula	m/z	Observed M/Z	Difference_Da	Difference_PPM	Score
C27 H19 B F2 N4 O S	497.1416	497.141596502698	0.111301442814238	0.22478886722732	97.97

Compound Spectra (Zoomed)



MassHunter Qual 10.0
(End of Report)

Figure S13. HR mass spectrum of compound **4**

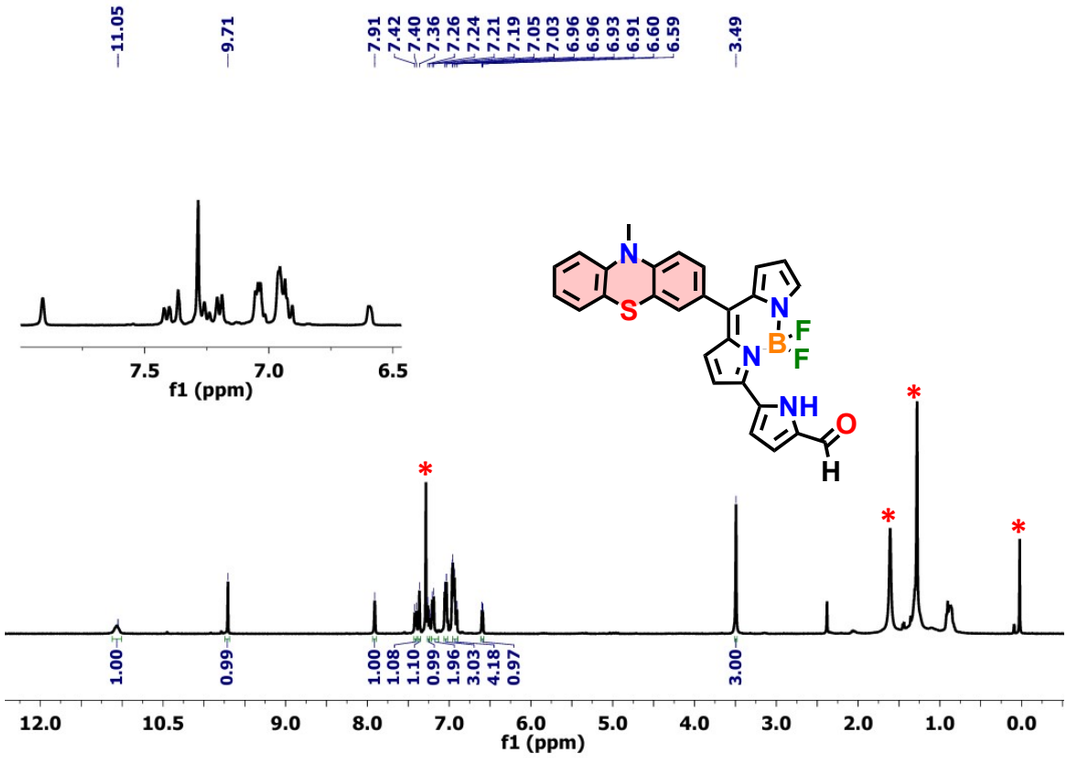


Figure S14. ^{1}H NMR spectrum of the compound **4** recorded in $CDCl_3$ on 400 MHz NMR instrument. The expansion of the aromatic region is shown in the inset. Note: Peaks marked with an asterisk (*) are due to residual solvents.

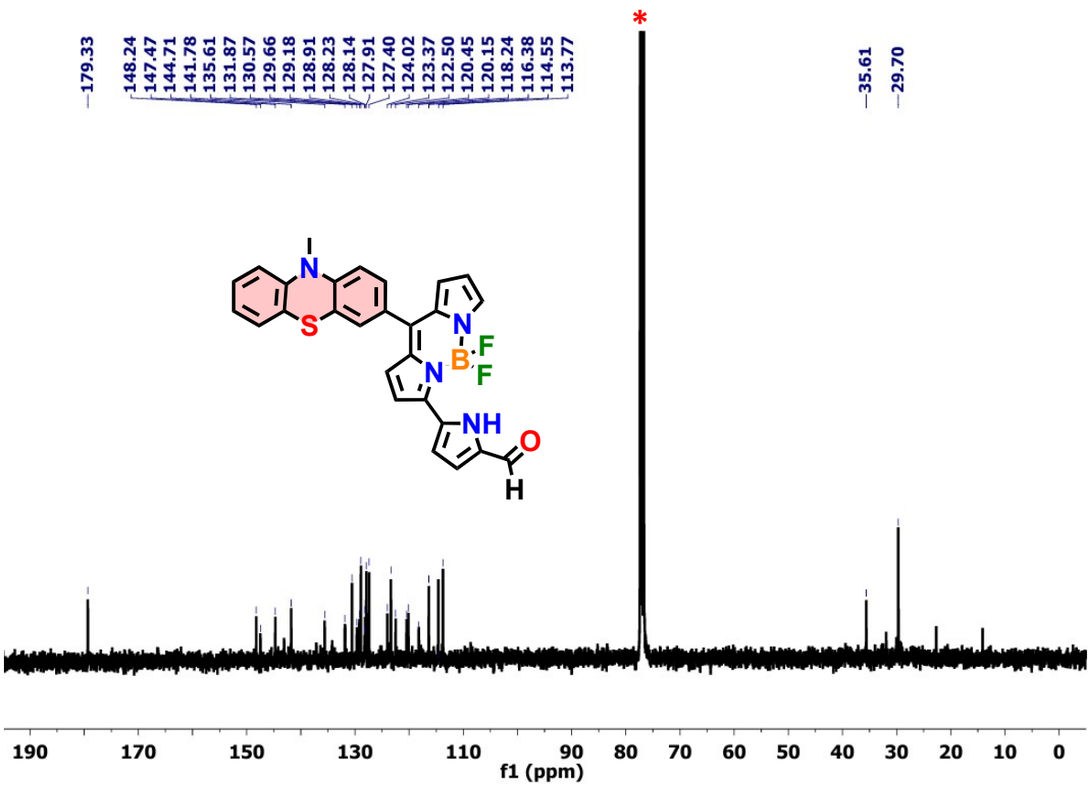


Figure S15. $^{13}C\{1H\}$ NMR spectrum of the compound **4** recorded in $CDCl_3$ on 100.06 MHz NMR instrument; Note: Peaks marked with an asterisk (*) are due to residual solvents.

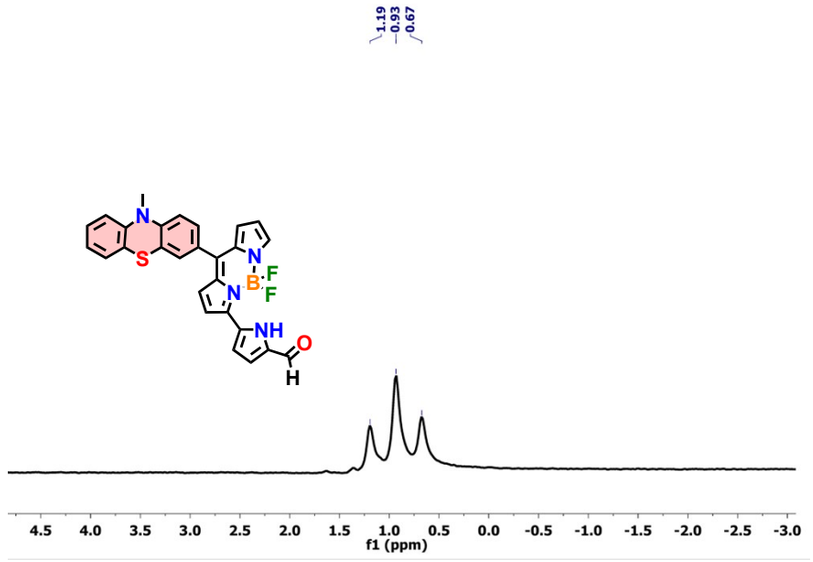


Figure S16. ^{11}B NMR spectrum of the compound **4** recorded in $CDCl_3$.

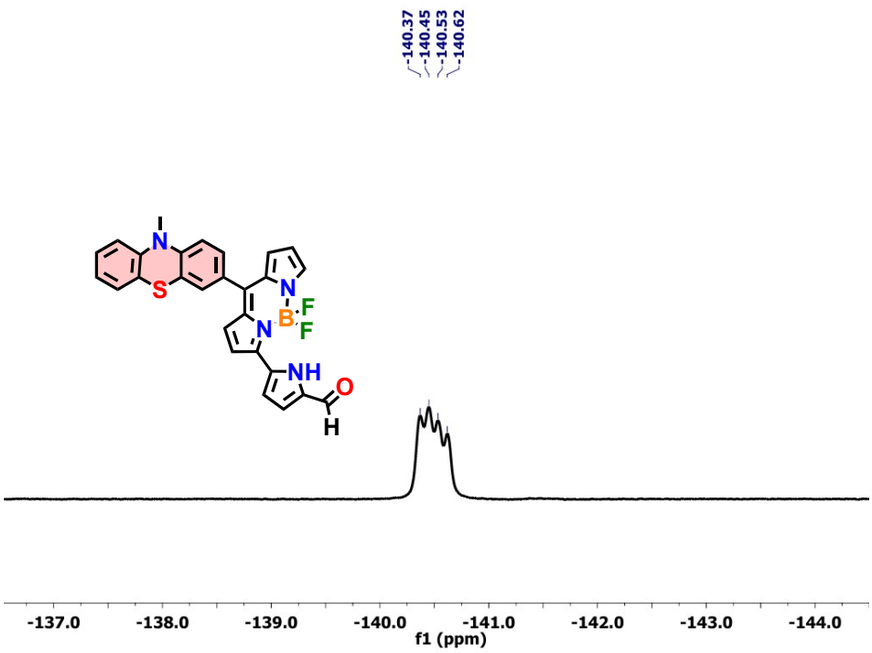
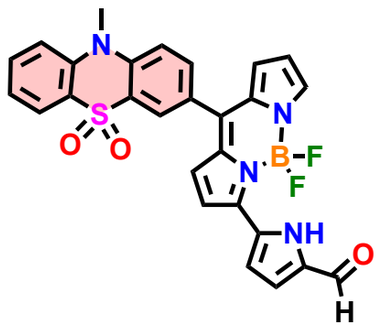


Figure S17. ^{19}F NMR spectrum of the compound **4** recorded in $CDCl_3$



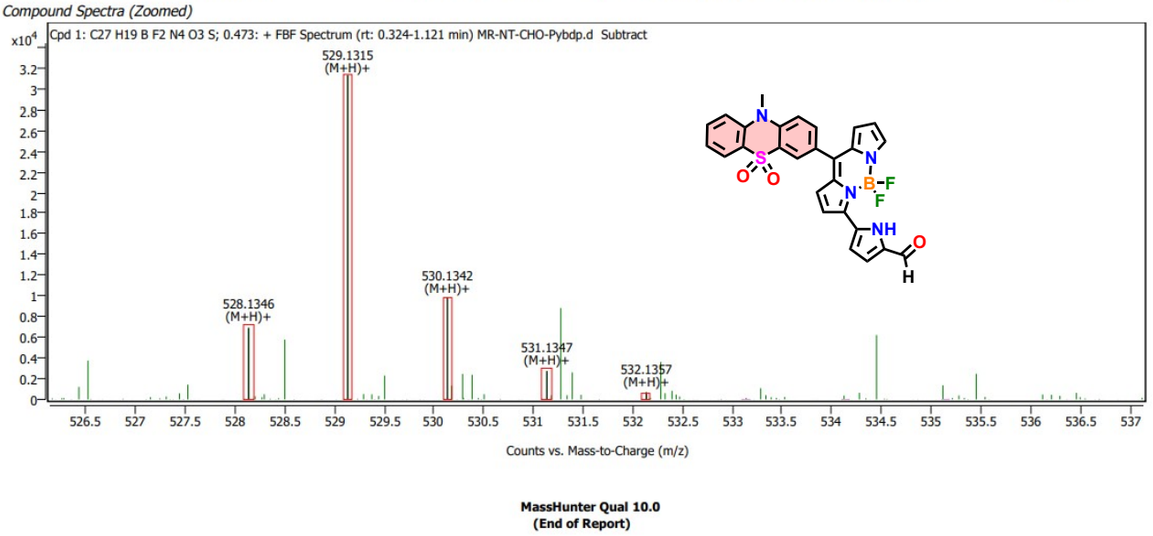
Compound 4.SO_2

Compound Details

Cpd. 1: C27 H19 B F2 N4 O3 S

Formula	m/z	Observed M/Z	Difference_Da	Difference_PPM	Score
C27 H19 B F2 N4 O3 S	529.1315	529.131488423223	-0.0207503036335766	-0.0393648642181574	99.76

Compound Spectra (Zoomed)



MassHunter Qual 10.0
(End of Report)

Figure S18. HR mass spectrum of compound **4.SO_2.**

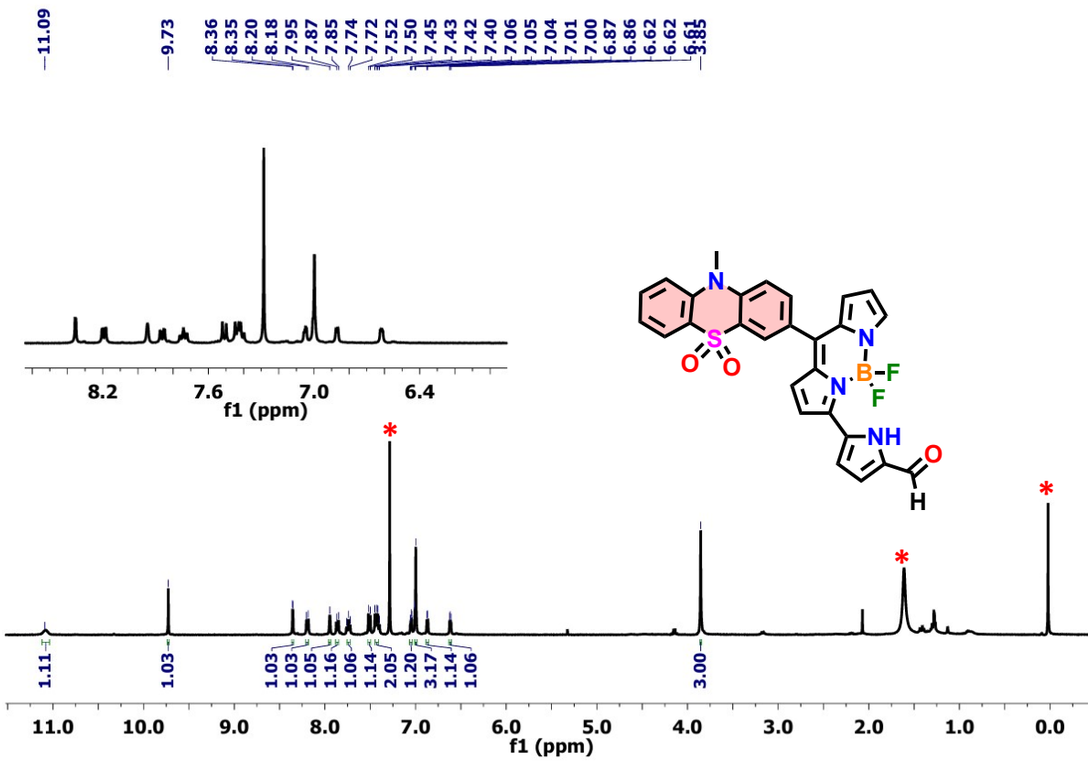


Figure S19. ^{1}H NMR spectrum of the compound **4.SO$_2$** recorded in $CDCl_3$ on 400 MHz NMR instrument. The expansion of the aromatic region is shown in the inset. Note: Peaks marked with an asterisk (*) are due to residual solvents.

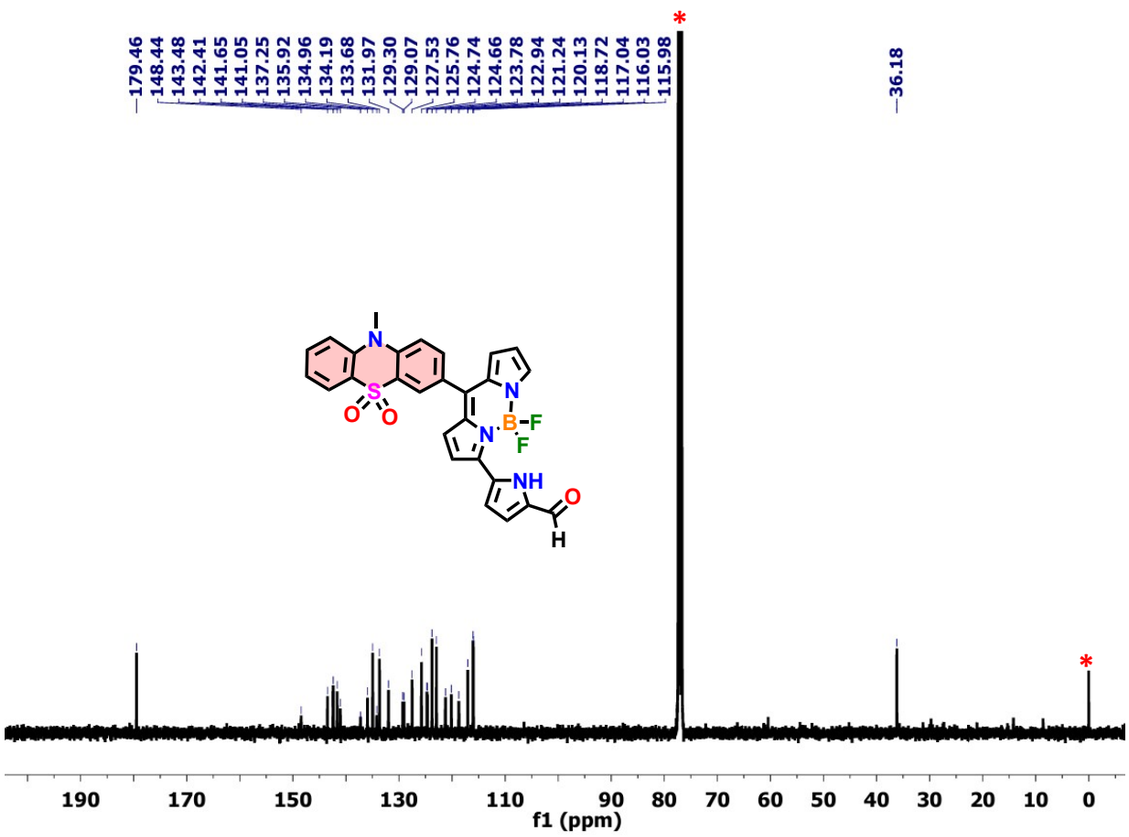


Figure S20. $^{13}C\{1H\}$ NMR spectrum of the compound **4.SO$_2$** recorded in $CDCl_3$ on 100.06 MHz NMR instrument; Note: Peaks marked with an asterisk (*) are due to residual solvents.

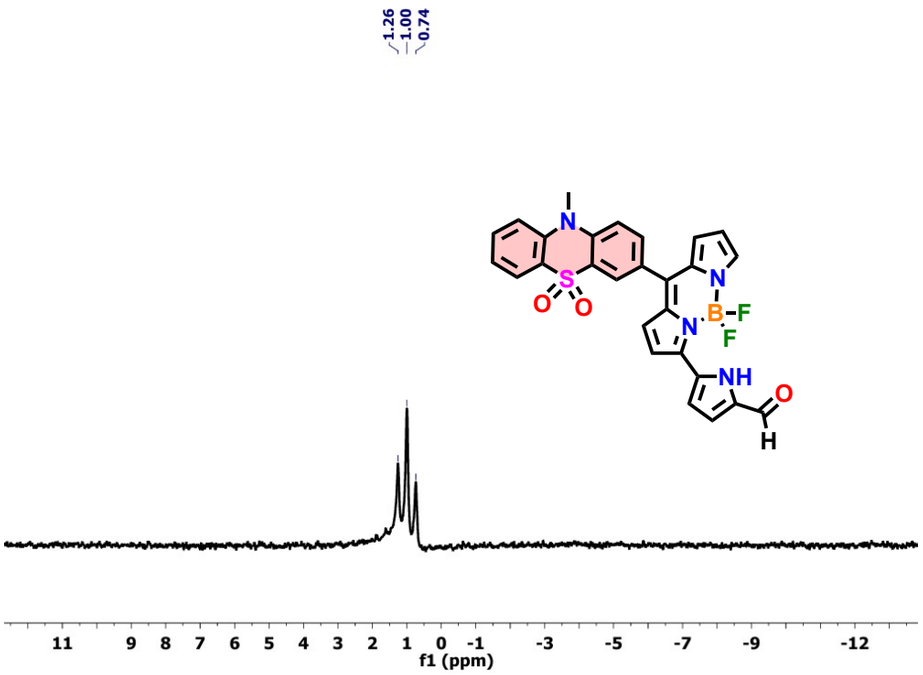


Figure S21. ^{11}B NMR spectrum of the compound **4.SO$_2$** recorded in $CDCl_3$.

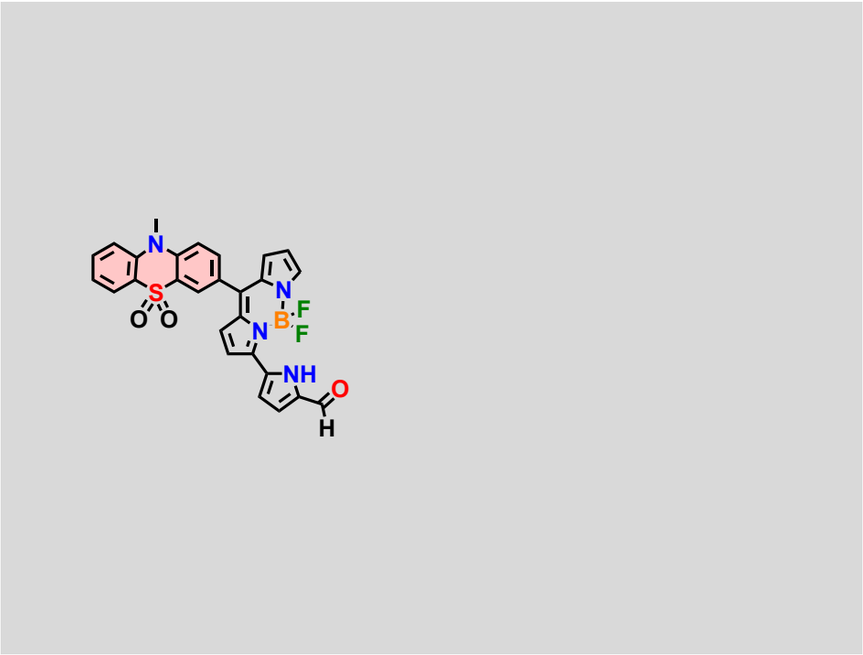
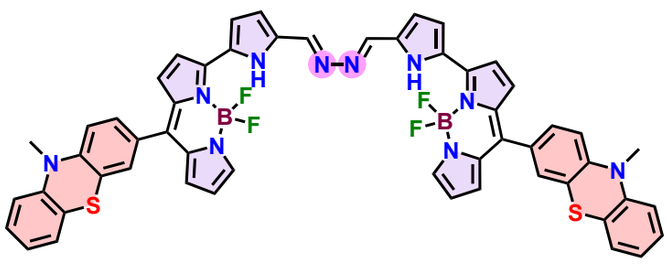


Figure S22. ^{19}F NMR spectrum of the compound **4.SO$_2$** recorded in $CDCl_3$



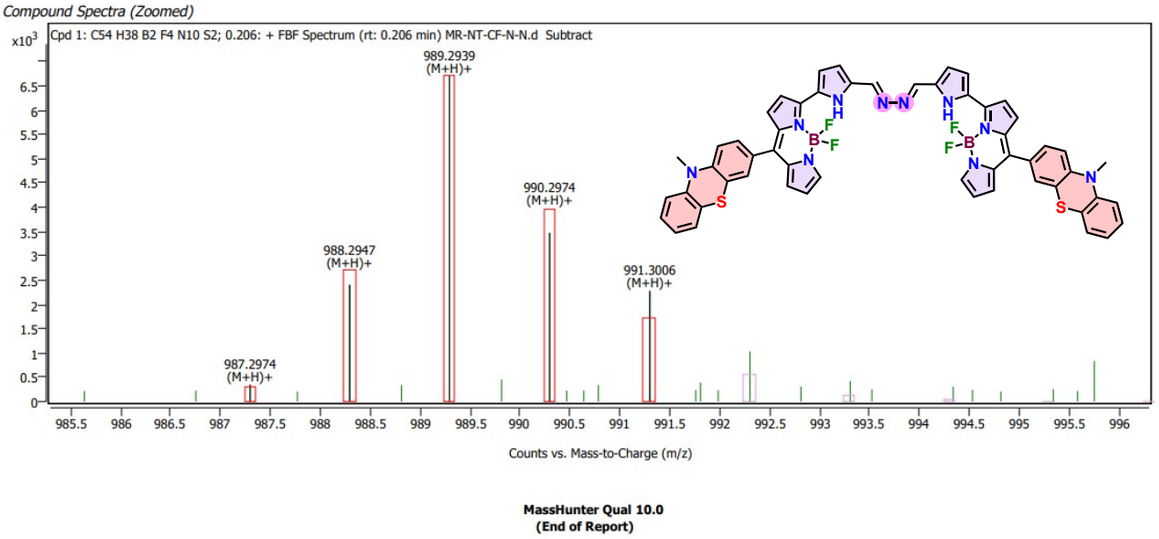
Compound 5

Compound Details

Cpd. 1: C54 H38 B2 F4 N10 S2

Formula	m/z	Observed M/Z	Difference_Da	Difference_PPM	Score
C54 H38 B2 F4 N10 S2	989.2939	989.293945851201	1.32377147883744	1.34217032581201	84.39

Compound Spectra (Zoomed)



MassHunter Qual 10.0
(End of Report)

Figure S23. HR mass spectrum of compound **5**

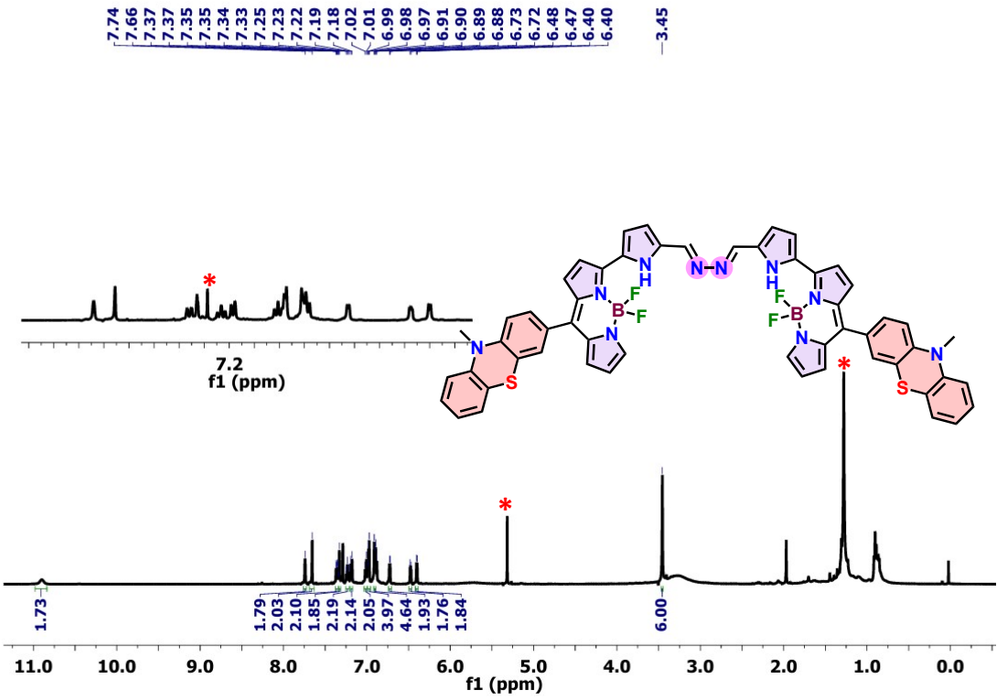


Figure S24. ^{1}H NMR spectrum of the compound **5** recorded in $CDCl_3$ on 400 MHz NMR instrument. The expansion of the aromatic region is shown in the inset. Note: Peaks marked with an asterisk (*) are due to residual solvents.

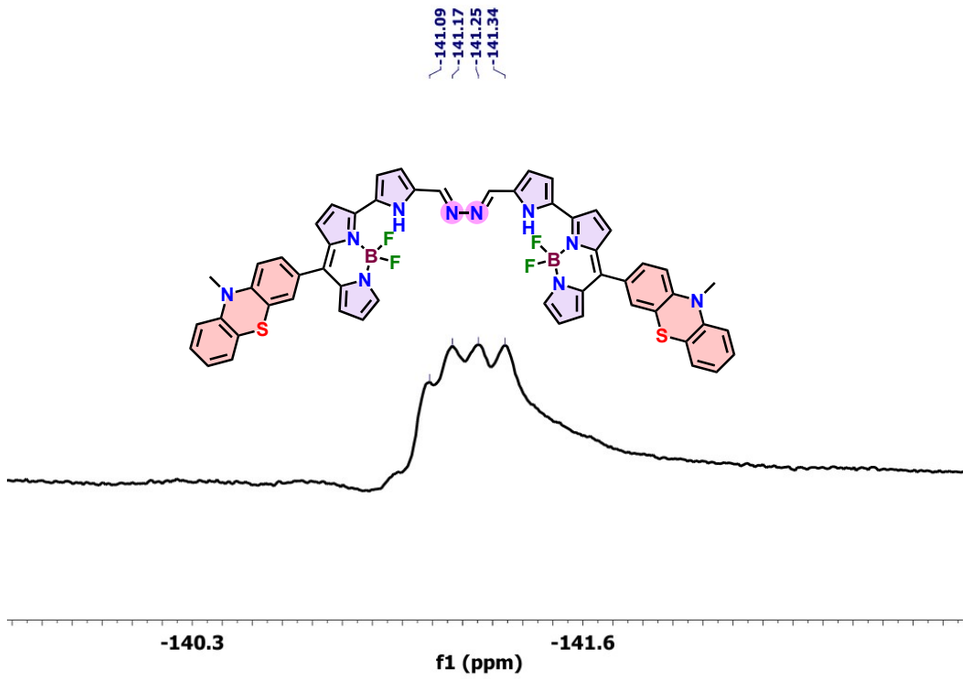


Figure S25. ^{19}F NMR spectrum of the compound **5** recorded in $CDCl_3$.

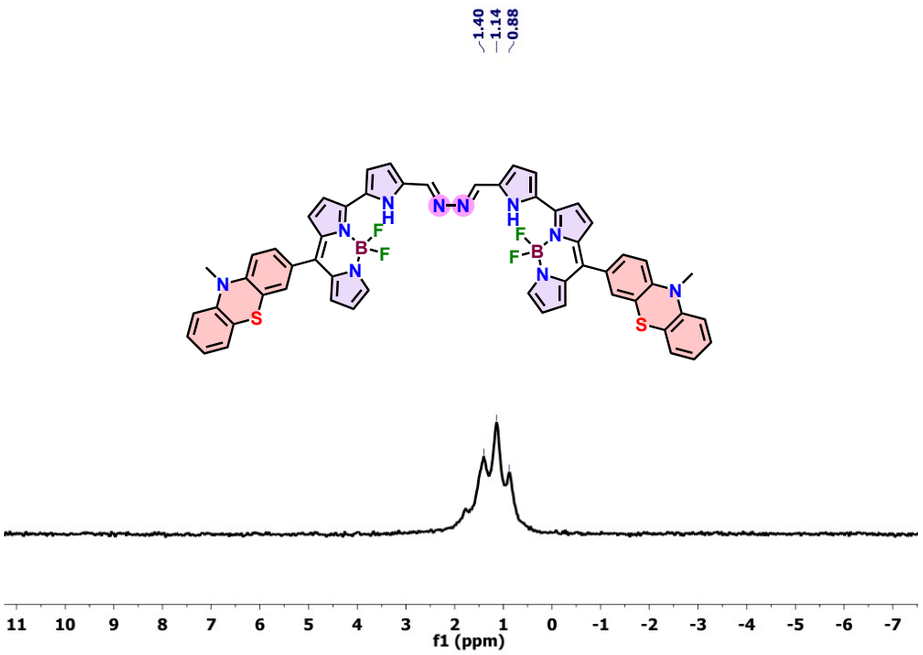
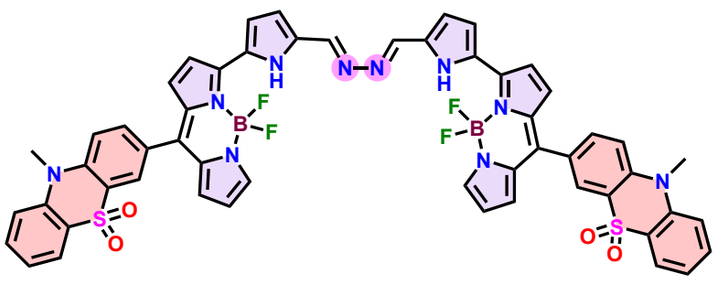


Figure S26. ^{11}B NMR spectrum of the compound **5** recorded in $CDCl_3$



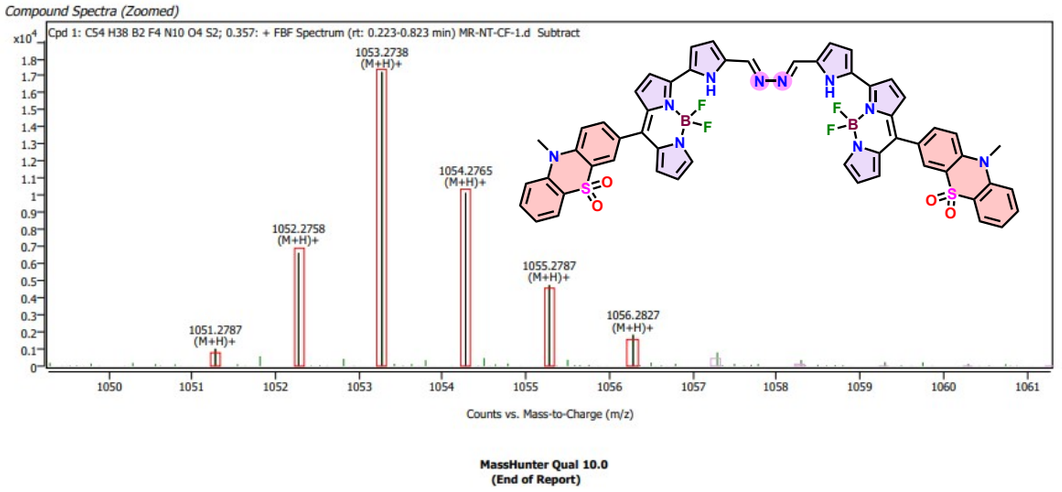
Compound 5.SO_2

Compound Details

Cpd. 1: C54 H38 B2 F4 N10 O4 S2

Formula	m/z	Observed M/Z	Difference_Da	Difference_PPM	Score
C54 H38 B2 F4 N10 O4 S2	1053.2738	1053.2737630097	1.46136961529919	1.39142096565032	97.08

Compound Spectra (Zoomed)



MassHunter Qual 10.0
(End of Report)

Figure S27. HR mass spectrum of compound **5.SO_2**

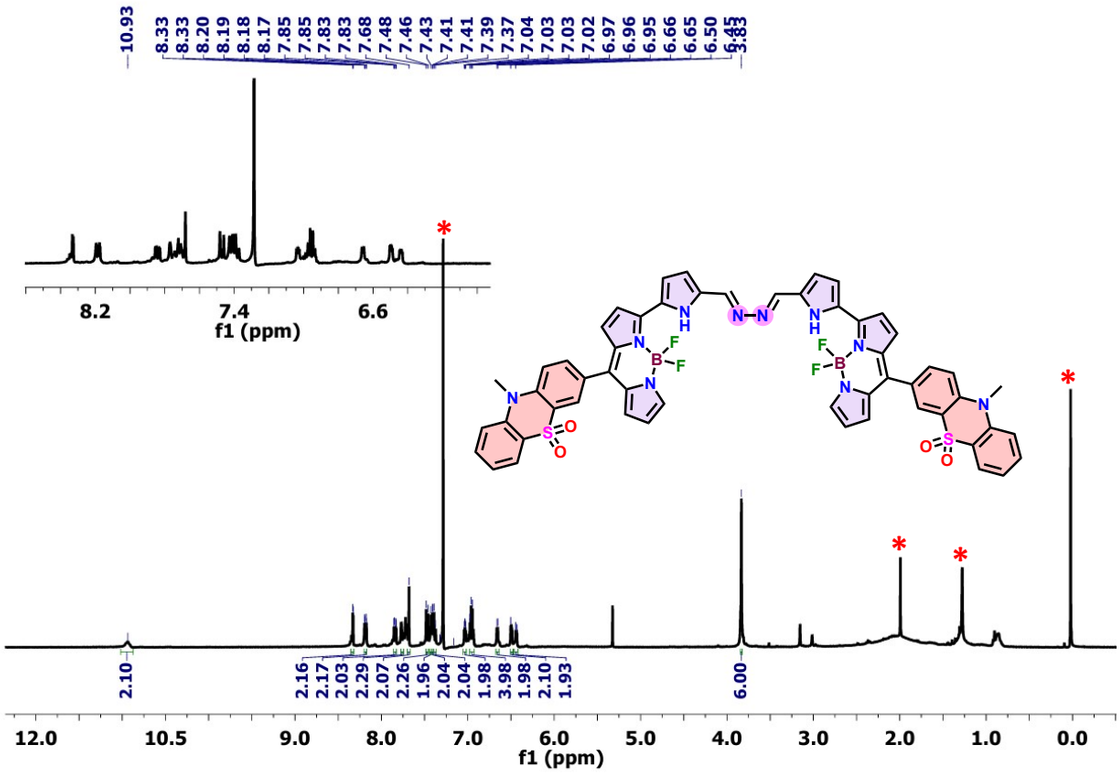


Figure S28. ^{1}H NMR spectrum of the compound **5.SO$_2$** recorded in $CDCl_3$ on 400 MHz NMR instrument. The expansion of the aromatic region is shown in the inset. Note: Peaks marked with an asterisk (*) are due to residual solvents.

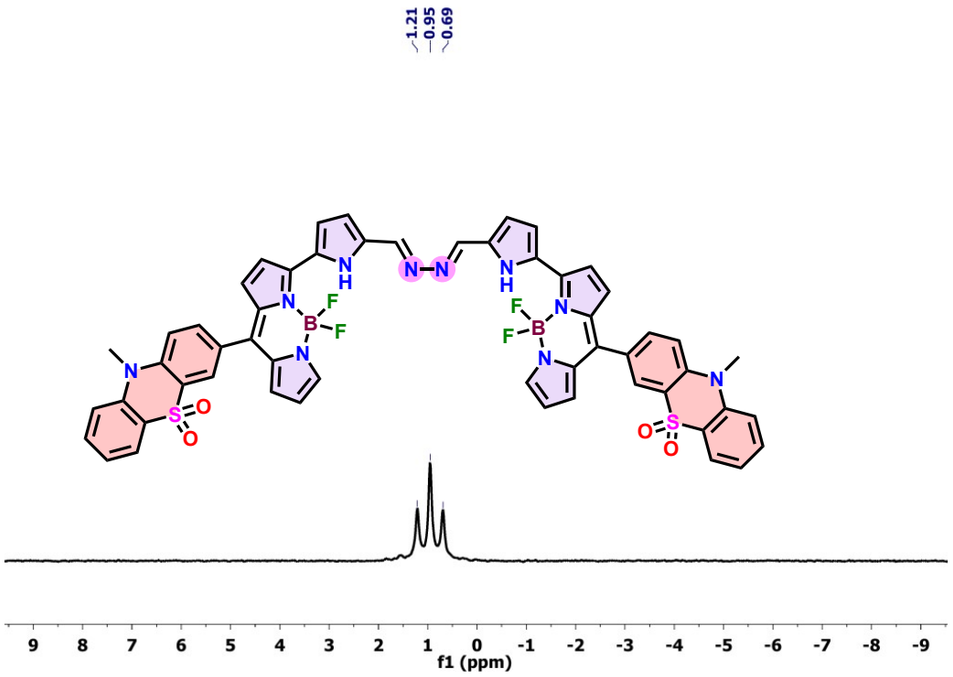


Figure S29. ^{11}B NMR spectrum of the compound **5.SO$_2$** recorded in $CDCl_3$.

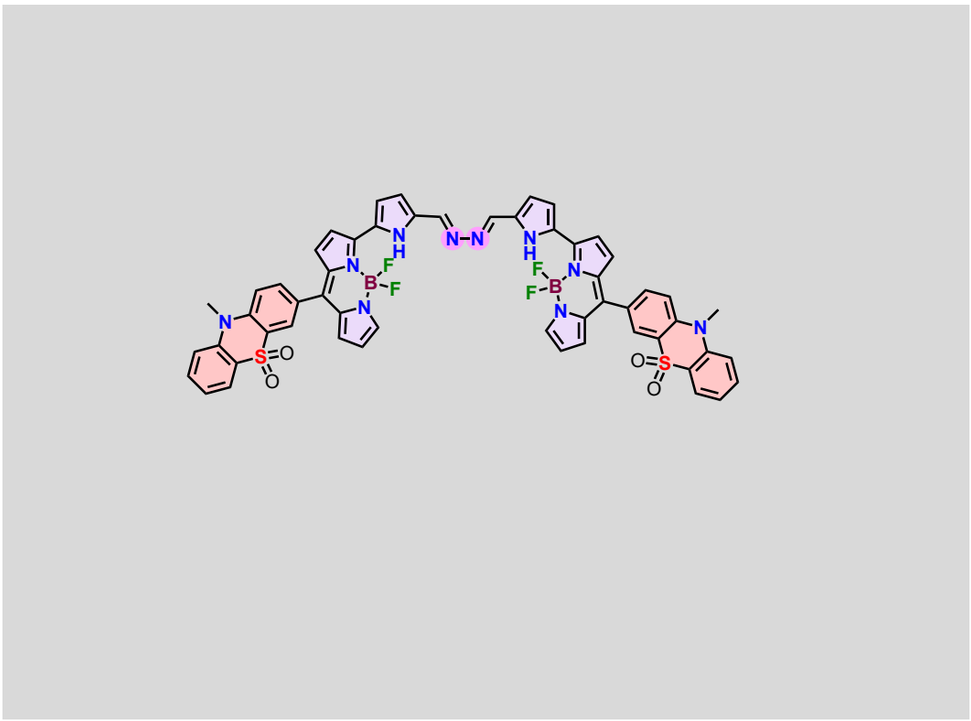
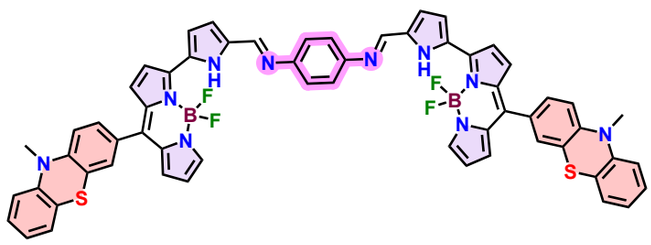


Figure S30. ^{19}F NMR spectrum of the compound **5.SO$_2$** recorded in $CDCl_3$



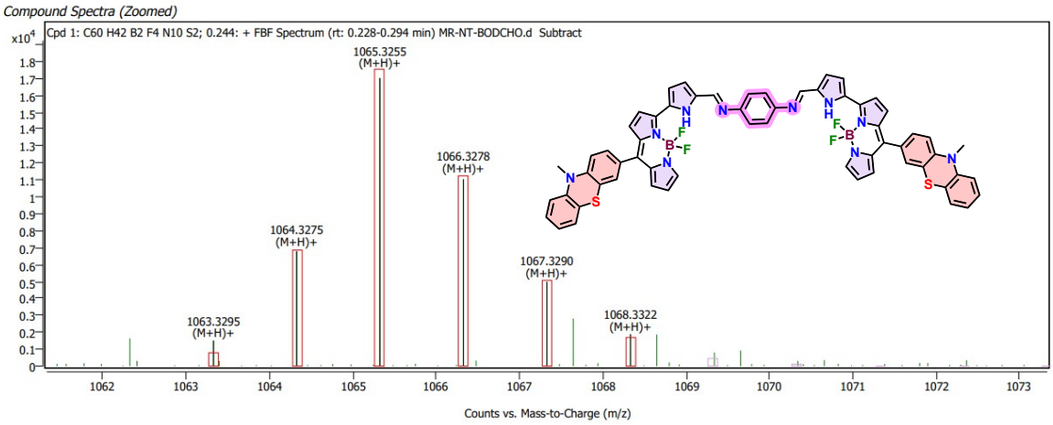
Compound 6

Compound Details

Cpd. 1: C60 H42 B2 F4 N10 S2

Formula	m/z	Observed M/Z	Difference_Da	Difference_PPM	Score
C60 H42 B2 F4 N10 S2	1065.3255	1065.32549627897	0.97732750873547	0.91999089773238	97.58

Compound Spectra (Zoomed)



MassHunter Qual 10.0
(End of Report)

Figure S31. HR mass spectrum of compound **6**

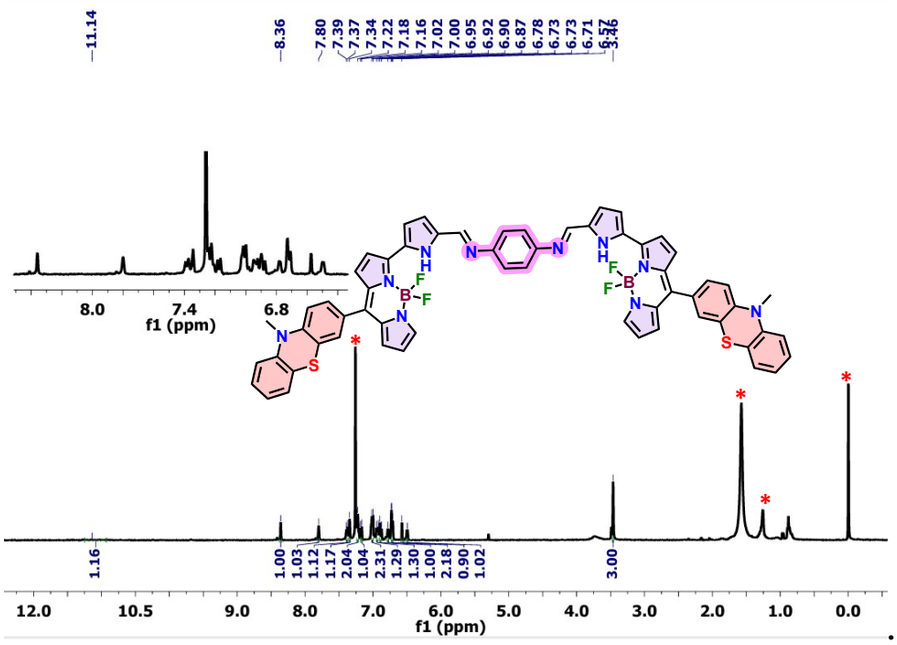


Figure S32. ^{1}H NMR spectrum of the compound **6** recorded in $CDCl_3$ on 400 MHz NMR instrument. The expansion of the aromatic region is shown in the inset. Note: Peaks marked with an asterisk (*) are due to residual solvents.

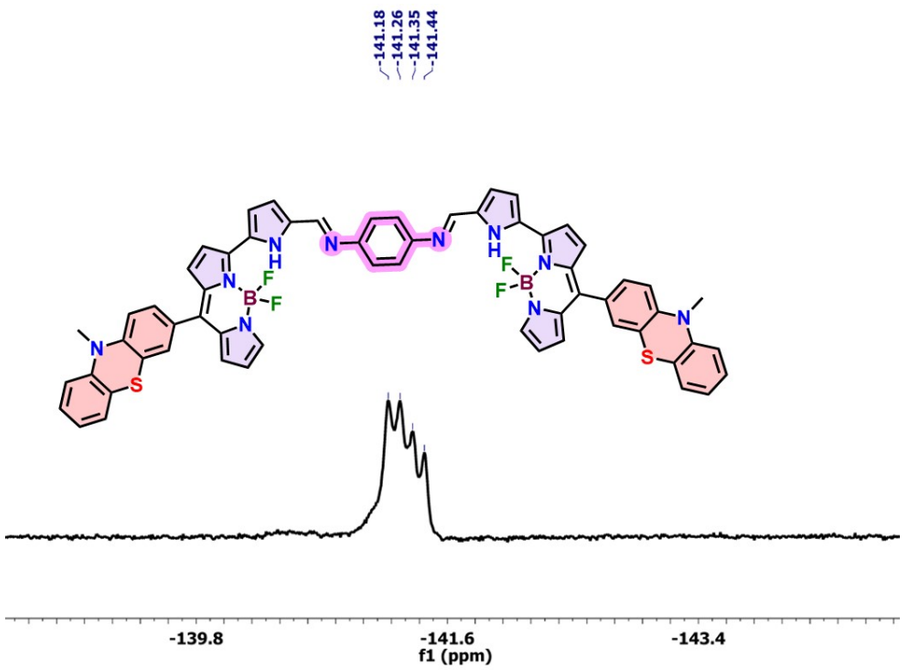


Figure S33. ^{19}F NMR spectrum of the compound **6** recorded in $CDCl_3$.

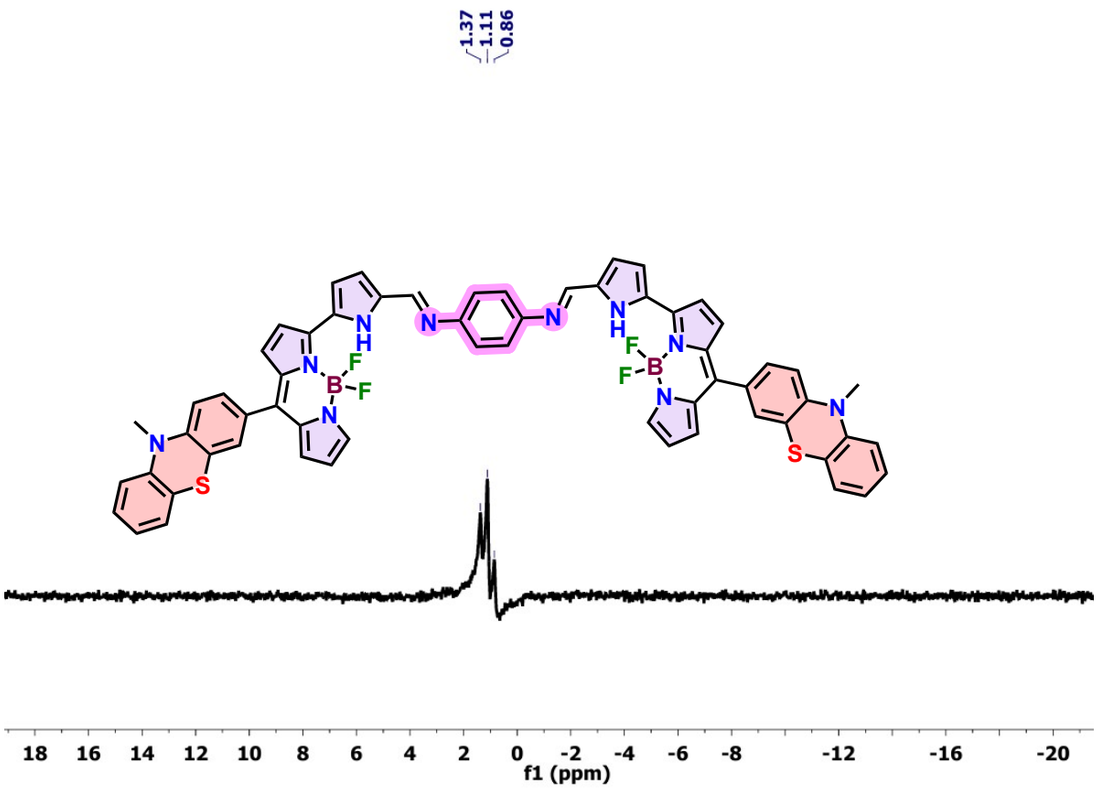
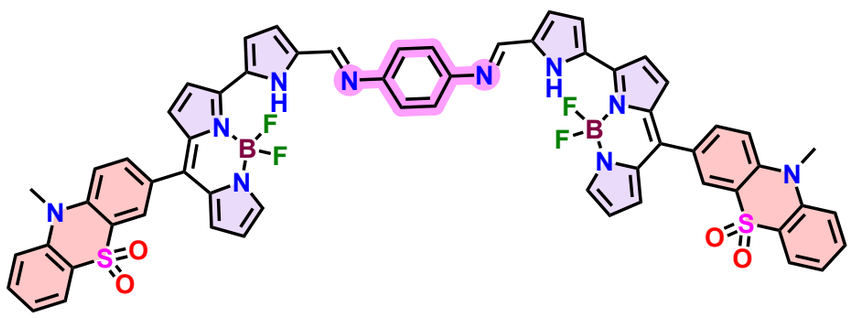


Figure S34. ^{11}B NMR spectrum of the compound **6** recorded in $CDCl_3$



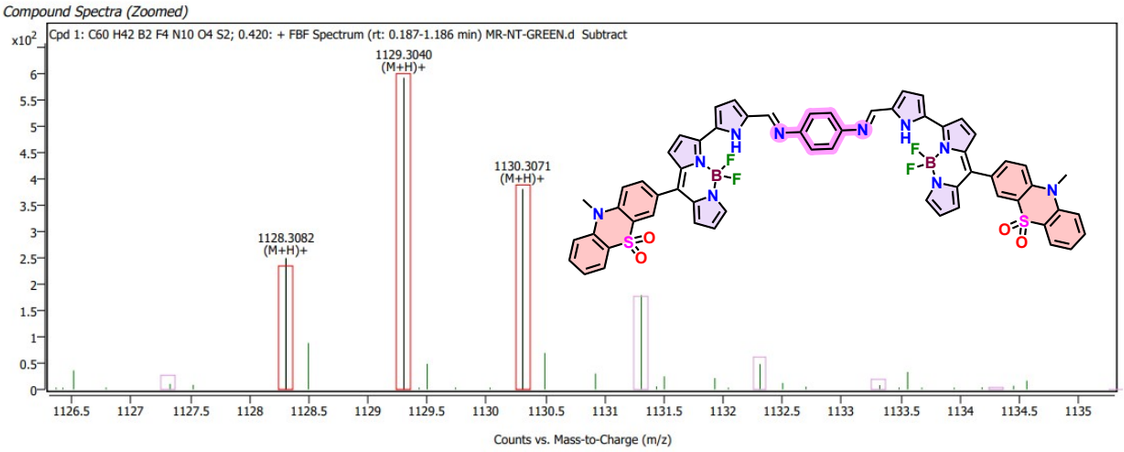
Compound 6.SO_2

Compound Details

Cpd. 1: C60 H42 B2 F4 N10 O4 S2

Formula	m/z	Observed M/Z	Difference_Da	Difference_PPM	Score
C60 H42 B2 F4 N10 O4 S2	1129.3040	1129.30404703507	0.228993354539853	0.203314223555499	69.01

Compound Spectra (Zoomed)



MassHunter Qual 10.0
(End of Report)

Figure S35. HR mass spectrum of compound **6.SO_2**

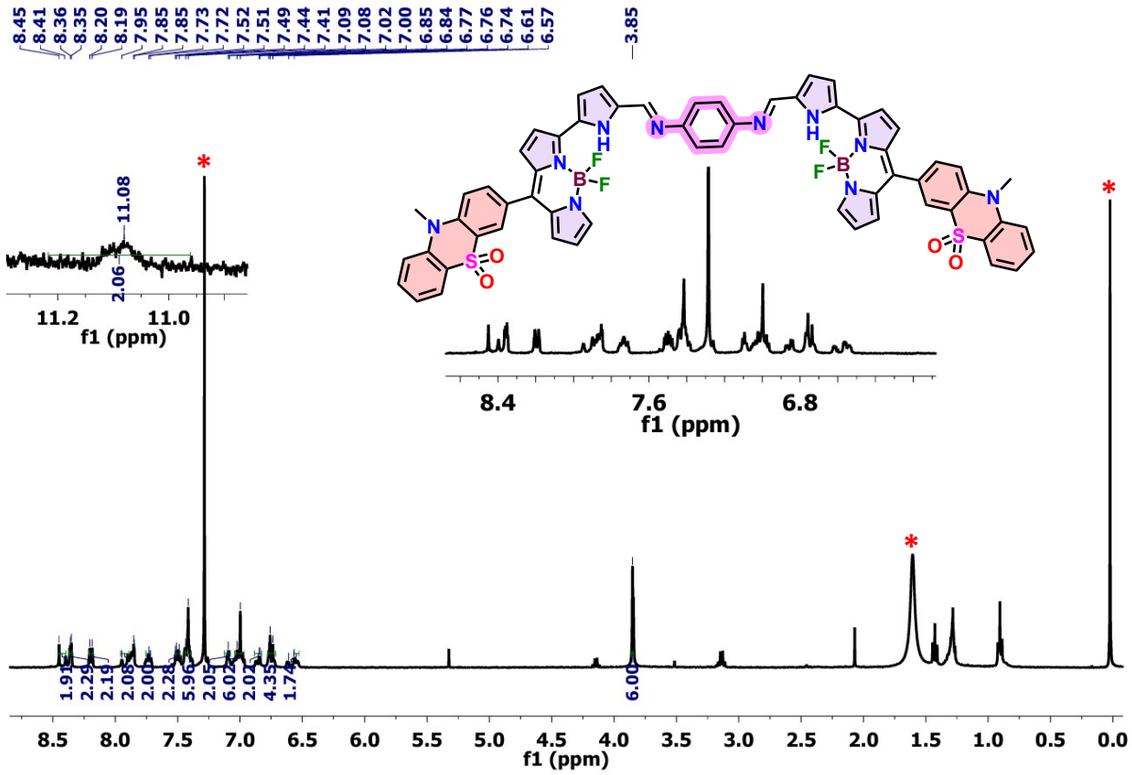
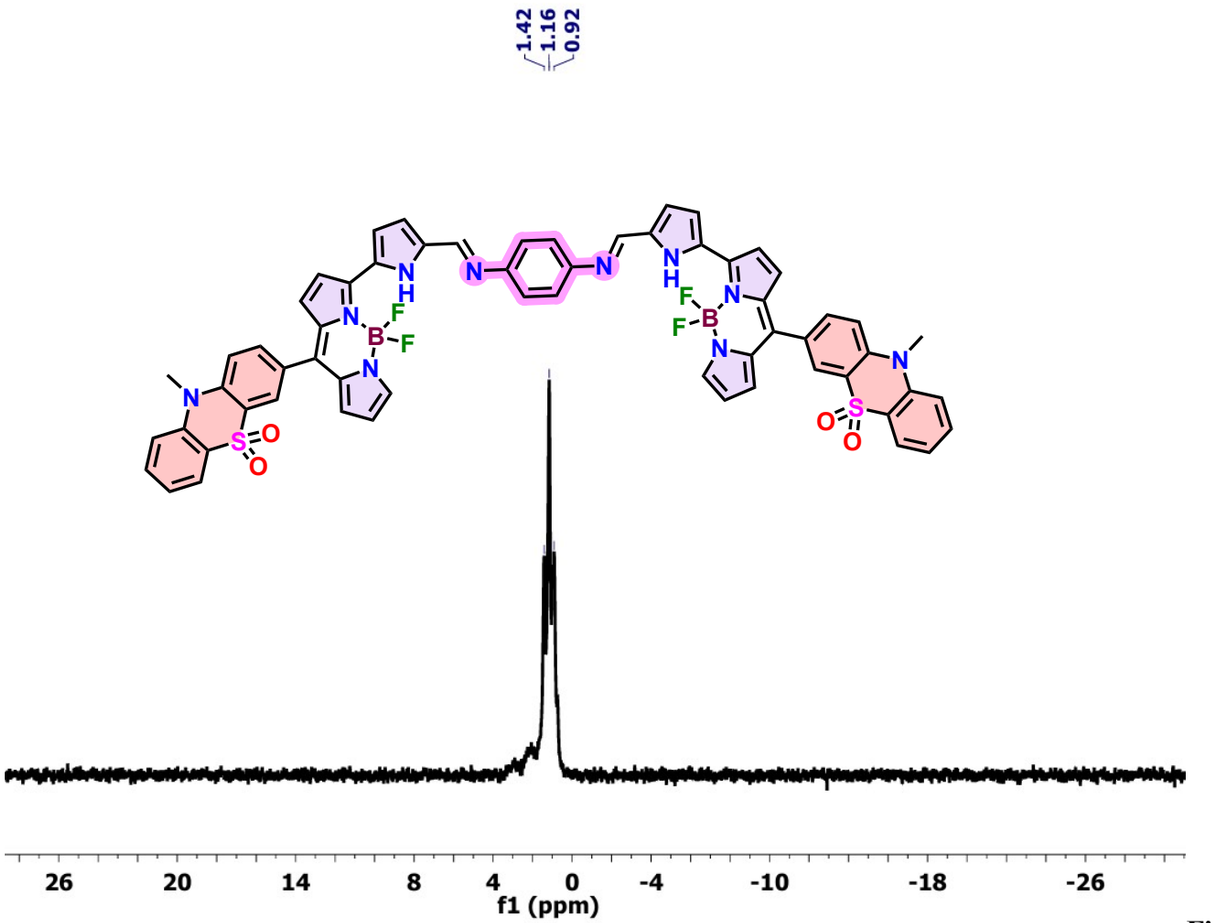


Figure S36. ^{1}H NMR spectrum of the compound **6.SO$_2$** recorded in $CDCl_3$ on 400 MHz NMR instrument. The expansion of the aromatic region is shown in the inset. Note: Peaks marked with an asterisk (*) are due to residual solvents.



Fi

gure S37. ^{11}B NMR spectrum of the compound **6.SO$_2$** recorded in $CDCl_3$.

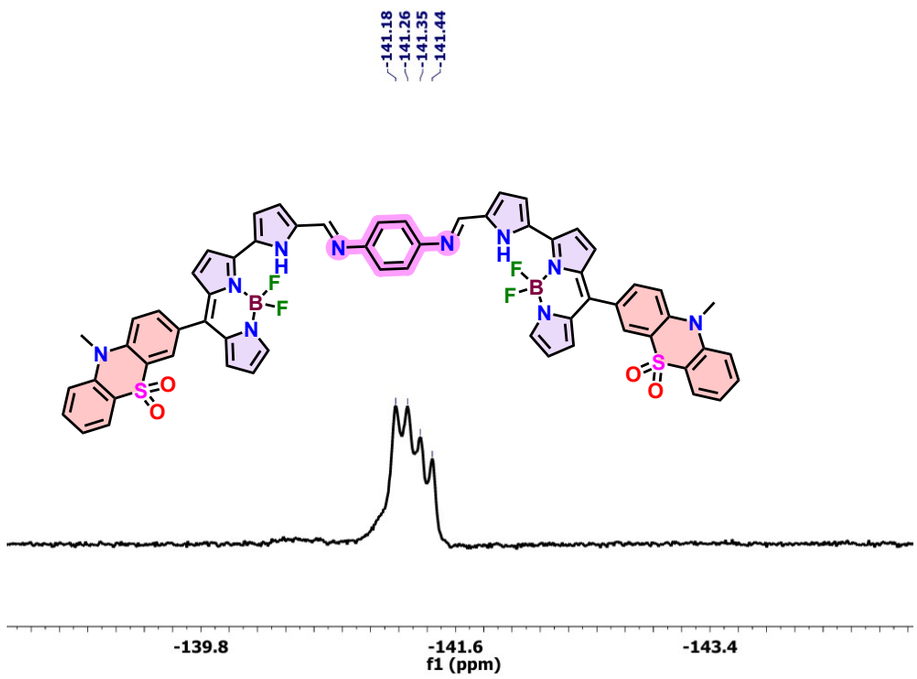


Figure S38. ^{19}F NMR spectrum of the compound **6.SO$_2$** recorded in $CDCl_3$

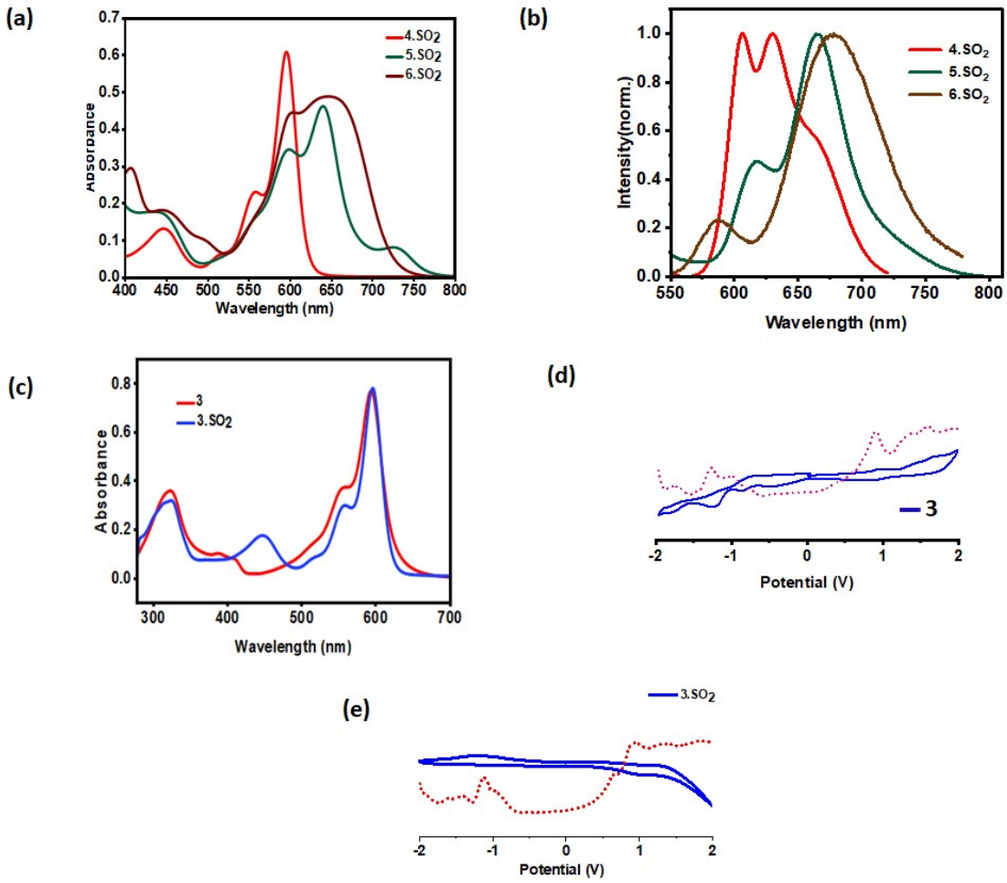
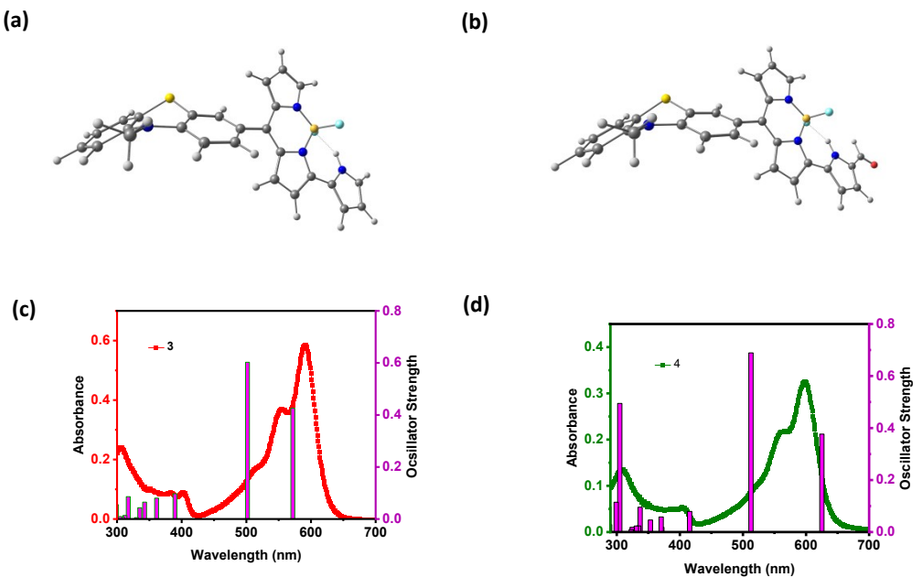
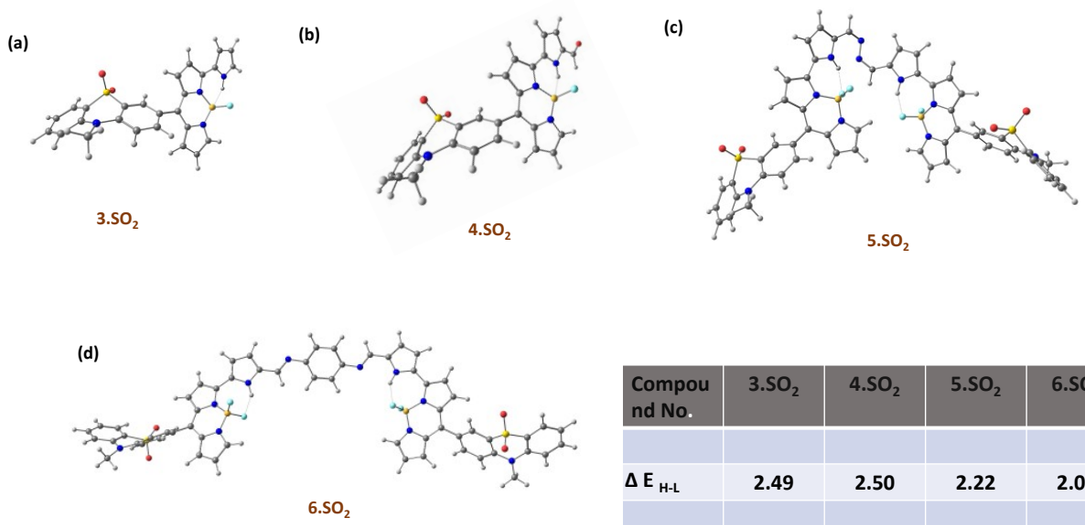


Figure 39. (a) Comparison of absorption spectra of compounds **4.SO$_2$**, **5.SO$_2$** and **6.SO$_2$** (1X10^{-5} M) recorded in toluene; (b) comparison of normalized emission spectra of compounds **4.SO$_2$**, **5.SO$_2$** and **6.SO$_2$** recorded in toluene; (c) Comparison of absorption spectra of compounds **3** and **3.SO$_2$** (1X10^{-5} M) recorded in toluene; (d,e) Cyclic voltammogram and differential pulse voltammogram (dotted line) of compound **3** and **3.SO2** recorded in CH_2Cl_2 containing 0.1 M tetrabutylammonium perchlorate (TBAP) as the supporting electrolyte and a saturated calomel electrode (SCE) as the reference electrode at a scan rate of 50 mV/s. A saturated calomel electrode (SCE) was employed as the reference electrode, glassy carbon as the working electrode, and platinum wire as the auxiliary electrode. (Note that polarographic convention has been followed for plotting CV starting at 0 V.)



Compound No.	3	4	5	6
$\Delta E_{H\text{-}L}$	2.48	2.40	2.27	2.04

Figure S40. (a) Optimized structures of *meso*-phenothiazinyl 3-pyrrolyl-BODIPY **3**, (b) *α*-formyl *meso*-phenothiazinyl 3-pyrrolyl-BODIPY **4**, (c) Calculated excitations (pink vertical lines) and experimental UV/vis absorption spectra (red line) for Schiff base **3** (ε in M^{-1} cm^{-1}); (d) Calculated excitations (pink vertical lines) and experimental UV/vis absorption spectra (green line) for Schiff base **4** (ε in M^{-1} cm^{-1}); Table showing the HOMO-LUMO energy gaps of compounds **3-6** calculated at the B3LYP/6-31G(d,p) level of theory.



Compound No.	$3.SO_2$	$4.SO_2$	$5.SO_2$	$6.SO_2$
ΔE_{H-L}	2.49	2.50	2.22	2.06

Figure S41. (a) Optimized structures of *meso*-phenothiazinyl-5,5 dioxide 3-pyrrolyl-BODIPY **3.SO₂**, (b) *α*-formyl *meso*-phenothiazinyl-5,5 dioxide 3-pyrrolyl-BODIPY **4.SO₂**, (c) Schiff base dyad derivative *bis*(*meso*-phenothiazinyl-5,5 dioxide - 3-pyrrolyl BODIPY)s **5.SO₂**, (d) Schiff base dyad derivative *bis*(*meso*-phenothiazinyl-5,5 dioxide - 3-pyrrolyl BODIPY)s **6.SO₂** calculated by the B3LYP /6-31G (d, p) method. Table showing the HOMO-LUMO energy gaps of compounds **3.SO₂-6.SO₂** calculated at the B3LYP/6-31G(d,p) level of theory.

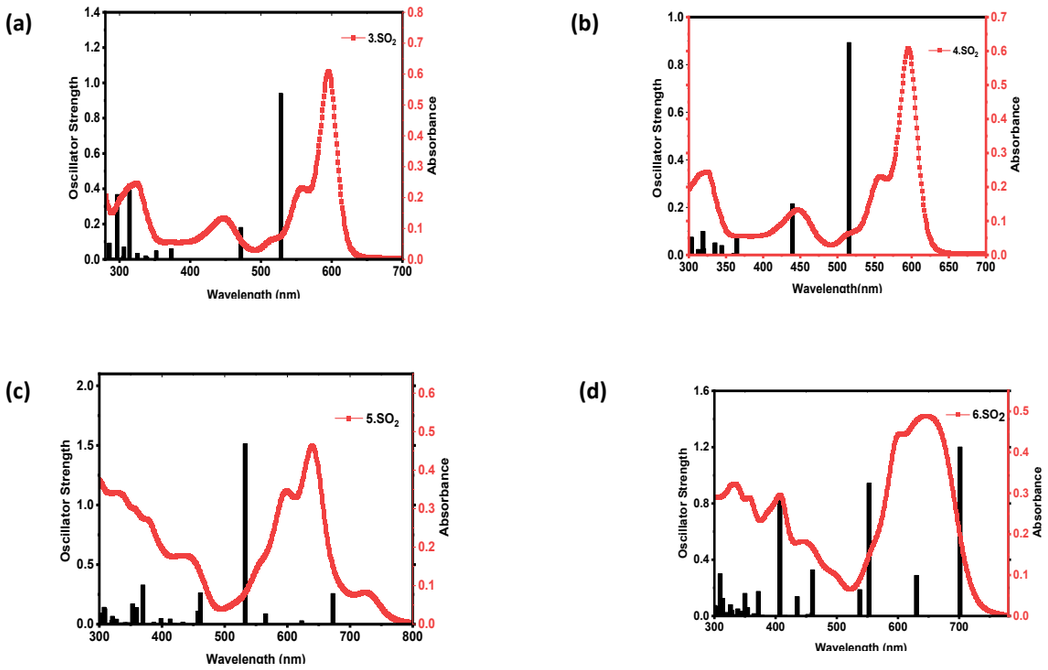


Figure S42. (a-d) Calculated excitations (black vertical lines) and experimental UV/vis absorption spectra (red line) for *meso*-phenothiazinyl-5,5 dioxide 3-pyrrolyl-BODIPY **3.SO₂,** *α*-formyl *meso*-phenothiazinyl-5,5 dioxide 3-pyrrolyl-BODIPY **4.SO₂**, Schiff base dyad derivative *bis*(*meso*-phenothiazinyl-5,5 dioxide - 3-pyrrolyl BODIPY)s **5.SO₂**, Schiff base dyad derivative *bis*(*meso*-phenothiazinyl-5,5 dioxide - 3-pyrrolyl BODIPY)s **6.SO₂** calculated by the B3LYP /6-31G (d, p) method. (ε in M^{-1} cm^{-1})

Table S1. Selected TD-DFT calculated oscillator strengths and compositions of the major electronic transitions of **3**.

No.	Wavelength (nm)	Osc. Strength	Major contribs
1	571.909188672	0.4258	H-1->LUMO (39%), HOMO->LUMO (61%)
2	501.716546666	0.6026	H-1->LUMO (61%), HOMO->LUMO (40%)
3	389.642341333	0.0971	H-2->LUMO (97%)
4	361.206680298	0.0804	H-4->LUMO (25%), H-3->LUMO (66%)
5	342.64921792	0.065	H-4->LUMO (73%), H-3->LUMO (20%)
6	335.14676167	0.0434	H-5->LUMO (90%)
7	330.052423831	0.0052	H-1->L+1 (46%), HOMO->L+1 (47%)
8	317.338605099	0.086	H-8->LUMO (57%), H-7->LUMO (16%), H-6->LUMO (23%)
9	312.224107309	0.0139	H-8->LUMO (18%), H-6->LUMO (70%)
10	308.157759637	0.0078	H-8->LUMO (17%), H-7->LUMO (53%), HOMO->L+2 (15%)
11	304.472368096	0.0096	H-7->LUMO (15%), H-1->L+1 (29%), HOMO->L+1 (37%), HOMO->L+2 (13%)
12	298.908346422	0.0552	H-1->L+1 (16%), H-1->L+2 (21%), HOMO->L+2 (38%)
13	290.497172006	0.0236	H-1->L+2 (62%), HOMO->L+2 (22%), HOMO->L+3 (11%)
14	288.987234021	0.1184	H-1->L+3 (44%), HOMO->L+3 (36%)
15	268.085523725	0.0166	H-1->L+3 (44%), HOMO->L+3 (47%)
16	259.777888852	0.3031	HOMO->L+4 (86%)
17	255.880201866	0.4661	H-2->L+1 (11%), H-1->L+4 (35%), HOMO->L+5 (26%)
18	251.61683006	0.0529	H-2->L+1 (12%), H-1->L+4 (23%), HOMO->L+5 (53%)
19	248.714529613	0.0838	H-9->LUMO (41%), H-2->L+1 (22%), H-1->L+4 (24%)
20	246.764176841	0.0845	H-9->LUMO (39%), H-2->L+1 (21%)
21	245.037734717	0.0181	H-1->L+5 (71%), HOMO->L+5 (12%)
22	242.161356691	0.0462	H-2->L+1 (14%), H-1->L+6 (41%), HOMO->L+6 (29%)
23	238.128899881	0.0177	H-10->LUMO (68%)
24	234.44556579	0.0191	H-2->L+2 (79%)
25	228.803781303	0.0464	H-3->L+1 (78%)
26	225.192424237	0.0039	H-3->L+2 (16%), H-2->L+3 (66%)
27	222.421098635	0.0115	H-11->LUMO (16%), H-3->L+2 (46%), H-2->L+3 (19%)
28	221.979075827	0.0003	H-11->LUMO (53%), H-3->L+2 (12%), HOMO->L+7 (16%)
29	220.584968086	0.0098	H-1->L+6 (35%), HOMO->L+6 (57%)
30	219.577070773	0.0064	H-4->L+1 (59%)
31	218.059363699	0.0124	H-13->LUMO (52%)
32	217.749157892	0.0007	H-13->LUMO (34%), H-4->L+1 (16%)
33	215.643435103	0.0222	H-11->LUMO (13%), HOMO->L+7 (58%)
34	213.600125786	0.0427	H-4->L+2 (60%)

35	211.859117959	0.0043	H-7->L+1 (16%), H-4->L+2 (13%), H-2->L+4 (34%), H-2->L+5 (10%)
36	210.749945627	0.025	H-5->L+1 (29%), H-3->L+3 (22%), H-2->L+4 (13%)
37	210.317370379	0.0003	H-5->L+1 (43%)
38	209.083109348	0.0017	H-12->LUMO (84%)
39	208.362787396	0.0203	H-6->L+1 (12%), H-3->L+4 (10%), H-2->L+5 (17%), H-1->L+7 (17%)
40	206.867876351	0.0437	H-2->L+4 (22%), H-2->L+5 (24%), H-1->L+7 (28%)
41	206.726457711	0.037	H-3->L+4 (11%), H-1->L+7 (39%)
42	205.370447752	0.0167	H-6->L+2 (11%), H-5->L+2 (29%), H-3->L+3 (17%)
43	204.91900207	0.0438	H-7->L+1 (21%), H-6->L+1 (27%), H-3->L+3 (13%)
44	204.432451214	0.0223	H-8->L+1 (65%)
45	203.149535502	0.0012	H-6->L+2 (18%), H-5->L+2 (27%), H-3->L+4 (12%)
46	200.207003314	0.0269	H-4->L+3 (12%), H-4->L+4 (20%), H-3->L+4 (19%), HOMO->L+8 (11%)
47	199.858458012	0.0181	H-7->L+2 (27%), H-2->L+6 (30%)
48	199.543233998	0.0112	H-15->LUMO (12%), H-14->LUMO (15%), H-5->L+4 (10%), H-4->L+3 (21%)
49	198.985993792	0.052	H-15->LUMO (15%), H-14->LUMO (11%), H-8->L+2 (13%), H-4->L+3 (13%), H-2->L+6 (20%)
50	198.826442497	0.0121	H-15->LUMO (14%), H-8->L+2 (26%), HOMO->L+9 (10%)

Table S2. Selected TD-DFT calculated oscillator strengths and compositions of the major electronic transitions of **3.SO_2**.

No.	Wavelength (nm)	Osc. Strength	Major contribs
1	515.655435918	0.8927	HOMO->LUMO (99%)
2	439.488827097	0.2153	H-1->LUMO (97%)
3	364.616495154	0.0734	H-4->LUMO (12%), H-3->LUMO (19%), H-2->LUMO (64%)
4	360.36678684	0.0067	HOMO->L+1 (97%)
5	344.171088753	0.0397	H-3->LUMO (79%), H-2->LUMO (12%)
6	335.264576437	0.0509	H-4->LUMO (78%), H-2->LUMO (13%)
7	320.033538144	0.0268	HOMO->L+2 (92%)
8	319.119203676	0.0991	H-6->LUMO (71%), H-5->LUMO (20%)
9	312.720238637	0.023	H-6->LUMO (12%), H-5->LUMO (23%), H-1->L+1 (54%)
10	303.436595723	0.0753	H-5->LUMO (44%), H-1->L+1 (36%)
11	293.884974429	0.0068	H-8->LUMO (18%), HOMO->L+3 (74%)
12	289.980805062	0.0243	H-8->LUMO (71%), HOMO->L+3 (20%)
13	287.900134709	0.0172	H-7->LUMO (89%)
14	280.342316764	0.2731	H-1->L+2 (89%)
15	264.33607584	0.0417	H-1->L+3 (13%), HOMO->L+4 (80%)

16	261.360497939	0.151	H-1->L+3 (74%)
17	256.680108921	0.353	H-9->LUMO (10%), HOMO->L+5 (67%)
18	256.57387375	0.0075	H-2->L+1 (89%)
19	253.515300806	0.0125	H-9->LUMO (88%)
20	245.226750949	0.0029	H-4->L+1 (28%), H-3->L+1 (67%)
21	240.470515356	0.0514	H-10->LUMO (80%)
22	236.160367642	0.0137	H-4->L+1 (13%), H-2->L+2 (59%)
23	235.58598657	0.0012	H-4->L+1 (50%), H-3->L+1 (20%), H-2->L+2 (23%)
24	233.452320722	0.0279	H-11->LUMO (26%), H-1->L+4 (53%)
25	232.73364183	0.0467	H-11->LUMO (55%), H-5->L+1 (15%)
26	231.603297055	0.1705	H-11->LUMO (14%), H-5->L+1 (30%), H-1->L+4 (22%)
27	228.163770725	0.0005	H-6->L+1 (79%), H-5->L+1 (13%)
28	226.269172392	0.0099	H-4->L+2 (24%), H-3->L+2 (58%)
29	225.24560899	0.0571	H-7->L+1 (54%), H-1->L+5 (13%)
30	224.637531956	0.0349	H-1->L+5 (73%)
31	222.317403956	0.0024	H-2->L+3 (65%)
32	220.651704951	0.0099	H-12->LUMO (78%)
33	219.974438927	0.1615	H-8->L+1 (58%)
34	219.324594042	0.0082	H-15->LUMO (69%), H-14->LUMO (13%), H-12->LUMO (12%)
35	218.289716209	0.001	H-4->L+2 (61%), H-3->L+2 (26%)
36	217.040162822	0.0057	H-13->LUMO (47%), HOMO->L+6 (35%)
37	215.684700112	0.0339	H-7->L+2 (16%), H-5->L+2 (15%), H-5->L+3 (12%), H-2->L+3 (22%)
38	213.924449182	0.0301	H-13->LUMO (34%), H-9->L+1 (11%), HOMO->L+6 (26%)
39	213.533908018	0.0022	H-9->L+1 (79%)
40	211.202291176	0.0017	H-6->L+2 (69%), H-5->L+2 (10%)
41	211.148338719	0.0105	H-4->L+3 (20%), H-3->L+3 (64%)
42	208.055096342	0.0282	H-5->L+2 (24%), H-2->L+4 (21%), H-2->L+5 (22%)
43	207.324492512	0.0439	H-14->LUMO (11%), H-6->L+2 (13%), H-5->L+2 (20%)
44	206.162711406	0.0943	H-14->LUMO (16%), H-8->L+2 (25%), H-2->L+4 (11%)
45	205.776062226	0.0183	H-14->LUMO (33%), H-4->L+3 (32%), H-3->L+3 (12%)
46	205.302434158	0.1296	H-14->LUMO (13%), H-8->L+2 (22%), H-7->L+2 (13%), H-4->L+3 (26%)
47	203.296100828	0.0428	H-2->L+4 (51%), H-2->L+5 (22%)
48	200.793873406	0.0222	H-16->LUMO (39%), H-3->L+4 (13%), H-3->L+5 (21%)
49	200.268447257	0.0138	H-16->LUMO (56%), H-3->L+5 (13%)
50	198.98918743	0.0009	H-6->L+3 (71%), H-5->L+3 (12%)

Table S3. Selected TD-DFT calculated oscillator strengths and compositions of the major electronic transitions of **4**.

No.	Wavelength (nm)	Osc. Strength	Major contribs
1	625.172413333	0.3765	HOMO->LUMO (97%)
2	512.755140663	0.689	H-1->LUMO (98%)
3	415.552329442	0.0795	H-2->LUMO (97%)
4	371.465958631	0.018	H-4->LUMO (62%), H-4->L+1 (10%), H-3->LUMO (19%)
5	370.411666504	0.0582	H-5->LUMO (18%), H-4->LUMO (24%), H-3->LUMO (48%)
6	353.36219401	0.0464	H-5->LUMO (69%), H-3->LUMO (17%)
7	337.032628407	0.0954	H-6->LUMO (46%), HOMO->L+1 (29%), HOMO->L+2 (14%)
8	334.793813659	0.0238	H-7->LUMO (14%), H-6->LUMO (36%), HOMO->L+1 (26%), HOMO->L+2 (11%)
9	330.933385859	0.0233	H-9->LUMO (18%), H-7->LUMO (37%), H-1->L+1 (18%), HOMO->L+2 (18%)
10	327.575875221	0.0026	H-8->LUMO (17%), H-7->LUMO (14%), HOMO->L+1 (23%), HOMO->L+2 (31%)
11	324.404597222	0.0184	H-9->LUMO (57%), H-7->LUMO (18%), HOMO->L+2 (10%)
12	322.951194322	0.0098	H-9->LUMO (13%), H-8->LUMO (70%)
13	304.794220493	0.4947	H-6->LUMO (10%), H-1->L+1 (42%), HOMO->L+3 (19%)
14	299.088611502	0.1146	H-1->L+1 (15%), HOMO->L+3 (68%)
15	288.751672207	0.0285	H-1->L+2 (86%)
16	288.241486521	0.0059	H-4->LUMO (14%), H-4->L+1 (79%)
17	287.319690889	0.0975	HOMO->L+4 (82%)
18	276.836942375	0.0302	H-1->L+3 (87%)
19	259.288941197	0.0372	H-2->L+1 (93%)
20	258.602104564	0.0845	H-10->LUMO (84%)
21	254.838841183	0.0289	H-1->L+4 (45%), HOMO->L+5 (24%)
22	254.065969287	0.0381	H-11->LUMO (13%), H-1->L+4 (42%), HOMO->L+5 (29%)
23	249.781801906	0.3439	H-11->LUMO (18%), H-2->L+2 (38%), HOMO->L+5 (22%)
24	247.192202509	0.0288	H-3->L+1 (41%), H-2->L+2 (16%), HOMO->L+6 (13%)
25	246.205554256	0.0911	H-11->LUMO (37%), H-1->L+6 (10%), HOMO->L+6 (14%)
26	242.151897448	0.0603	H-3->L+1 (10%), H-2->L+2 (14%), HOMO->L+6 (12%), HOMO->L+7 (51%)

27	239.749764111	0.0144	H-3->L+1 (20%), HOMO->L+6 (35%), HOMO->L+7 (11%)
28	237.914134692	0.0041	H-6->L+1 (14%), H-1->L+5 (43%), HOMO->L+6 (16%)
29	236.01650996	0.0076	H-6->L+1 (12%), H-1->L+5 (34%), H-1->L+6 (25%)
30	234.952042851	0.0182	H-5->L+1 (55%), H-2->L+3 (30%)
31	234.631908354	0.0274	H-5->L+1 (33%), H-2->L+3 (47%)
32	231.720167854	0.0923	H-7->L+1 (33%), H-6->L+1 (18%), H-1->L+6 (39%)
33	226.877823547	0.031	H-12->LUMO (68%)
34	225.458599455	0.043	H-3->L+2 (43%), H-2->L+4 (11%)
35	225.08204381	0.0268	H-9->L+1 (78%)
36	223.548002258	0.001	H-3->L+2 (17%), H-2->L+4 (70%)
37	222.848862269	0.014	H-14->LUMO (16%), H-7->L+1 (31%), H-6->L+1 (33%)
38	221.693296521	0.0039	H-14->LUMO (73%)
39	219.448817679	0.006	H-8->L+1 (62%), H-3->L+2 (17%)
40	217.31787319	0.0145	H-8->L+1 (22%), H-3->L+3 (37%)
41	216.888293558	0.002	H-13->LUMO (56%)
42	215.639684521	0.014	H-13->LUMO (27%), H-5->L+2 (15%), H-3->L+3 (19%)
43	214.427618015	0.0145	H-5->L+2 (63%)
44	213.858030207	0.0041	HOMO->L+8 (86%)
45	211.739719942	0.0073	H-1->L+7 (83%), HOMO->L+7 (10%)
46	210.825201946	0.0012	H-8->L+2 (24%), H-5->L+3 (13%), H-2->L+5 (29%)
47	208.717056398	0.0583	H-8->L+2 (17%), H-5->L+3 (39%), H-2->L+5 (11%)
48	208.013208866	0.0073	H-5->L+3 (11%), H-4->L+2 (75%)
49	207.522291426	0.0202	H-6->L+2 (16%), H-5->L+3 (18%), H-4->L+2 (22%)
50	206.892040336	0.1058	H-1->L+8 (65%)

Table S4. Selected TD-DFT calculated oscillator strengths and compositions of the major electronic transitions of **4.SO_2**.

No.	Wavelength (nm)	Osc. Strength	Major contribs
1	528.244186495	0.9396	HOMO->LUMO (95%)
2	471.602103508	0.1803	H-1->LUMO (93%)
3	378.901635023	0.0005	H-3->LUMO (84%), H-3->L+2 (11%)
4	373.390131041	0.0601	H-4->LUMO (27%), H-2->LUMO (63%)
5	351.987829356	0.0474	H-4->LUMO (63%), H-2->LUMO (15%), HOMO->L+2 (13%)
6	338.76388156	0.0134	H-5->LUMO (75%), HOMO->L+1 (14%)
7	337.032628407	0.0196	H-5->LUMO (12%), HOMO->L+1 (77%)
8	331.180898609	0.0011	H-7->LUMO (77%)

9	325.477628468	0.0326	H-6->LUMO (69%)
10	314.162404693	0.3913	H-9->LUMO (18%), H-1->L+1 (22%), HOMO->L+2 (33%)
11	306.216979951	0.0701	H-8->LUMO (15%), H-6->LUMO (17%), H-1->L+1 (42%), HOMO->L+2 (11%)
12	305.319624242	0.0163	H-9->LUMO (40%), H-8->LUMO (29%), H-1->L+1 (21%)
13	303.08796297	0.0065	H-9->LUMO (22%), H-8->LUMO (34%), HOMO->L+3 (33%)
14	296.740685013	0.367	H-9->LUMO (10%), HOMO->L+2 (15%), HOMO->L+3 (54%)
15	290.279530371	0.0073	H-3->LUMO (13%), H-3->L+2 (73%)
16	285.816162226	0.0915	H-1->L+2 (69%), H-1->L+3 (21%)
17	277.18972705	0.0101	HOMO->L+4 (77%)
18	275.153557506	0.0852	H-1->L+2 (16%), H-1->L+3 (59%), HOMO->L+4 (16%)
19	266.197597501	0.0105	H-10->LUMO (99%)
20	261.217328949	0.1054	H-1->L+4 (87%)
21	250.579423619	0.0368	H-11->LUMO (22%), H-2->L+1 (14%), HOMO->L+5 (57%)
22	249.51036005	0.0274	H-11->LUMO (20%), H-2->L+1 (33%), HOMO->L+5 (38%)
23	248.306082296	0.0037	H-11->LUMO (32%), H-2->L+1 (45%), H-2->L+2 (12%)
24	246.088271629	0.0813	H-2->L+2 (48%), HOMO->L+6 (33%)
25	243.320955769	0.0002	H-12->LUMO (85%)
26	238.881339856	0.0085	H-4->L+1 (73%)
27	237.417550098	0.0499	H-5->L+2 (12%), H-4->L+1 (21%), H-4->L+2 (11%), H-2->L+2 (18%), HOMO->L+6 (13%)
28	234.060510491	0.0541	H-6->L+1 (20%), H-4->L+2 (61%)
29	233.795691223	0.2299	H-6->L+1 (14%), H-5->L+2 (44%), HOMO->L+6 (14%)
30	233.131873589	0.0007	H-3->L+1 (92%)
31	232.045428707	0.0273	H-2->L+3 (11%), H-1->L+5 (63%)
32	231.46925736	0.0544	H-6->L+1 (26%), H-4->L+2 (10%), HOMO->L+6 (13%)
33	229.885585842	0.0017	H-13->LUMO (90%)
34	227.694470382	0.004	H-7->L+1 (40%), H-5->L+1 (45%)
35	227.594157082	0.0267	H-2->L+3 (62%)
36	225.918719046	0.0563	H-8->L+1 (54%), H-6->L+1 (11%)
37	225.516011882	0.0278	H-7->L+2 (75%)
38	223.560094867	0.0	H-16->LUMO (94%)
39	223.105508192	0.0105	H-14->LUMO (77%)
40	222.728762642	0.0008	H-7->L+1 (43%), H-5->L+1 (38%)
41	221.538806419	0.016	H-6->L+2 (35%), H-6->L+4 (11%), H-2->L+4 (13%)
42	219.534303088	0.115	H-9->L+1 (45%), H-4->L+3 (26%)
43	218.282029951	0.0826	H-9->L+1 (13%), H-6->L+2 (12%), H-4->L+3 (51%)
44	217.348350418	0.0059	H-6->L+2 (35%), H-2->L+4 (19%)
45	216.2188152	0.0	H-3->L+3 (93%)

46	214.035239201	0.0042	H-15->LUMO (32%), H-10->L+1 (19%), H-1->L+6 (27%)
47	213.721631752	0.0142	H-10->L+1 (59%), H-1->L+6 (24%)
48	213.555976045	0.0116	H-15->LUMO (47%), H-1->L+6 (26%)
49	212.611151526	0.0064	H-8->L+2 (25%), H-2->L+4 (38%), H-1->L+6 (15%)
50	210.954337897	0.014	H-9->L+2 (11%), H-8->L+2 (30%), H-5->L+3 (12%), H-2->L+4 (10%)

Table S5. Selected TD-DFT calculated oscillator strengths and compositions of the major electronic transitions of **5**.

No.	Wavelength (nm)	Osc. Strength	Major contribs
1	662.946171598	0.031	HOMO->LUMO (97%)
2	629.042075151	0.2566	H-1->LUMO (53%), HOMO->L+1 (42%)
3	605.628140935	0.0287	H-1->L+1 (91%)
4	579.880234845	0.7257	H-3->LUMO (26%), H-2->L+1 (20%), H-1->LUMO (19%), HOMO->L+1 (30%)
5	553.352642204	0.1127	H-3->LUMO (51%), H-2->L+1 (41%)
6	527.659671499	0.003	H-2->LUMO (96%)
7	515.376784355	0.1245	H-3->L+1 (80%)
8	513.966724753	0.6753	H-3->LUMO (13%), H-3->L+1 (16%), H-2->L+1 (32%), H-1->LUMO (17%), HOMO->L+1 (20%)
9	412.003432733	0.0542	H-4->LUMO (87%)
10	400.789374534	0.2135	H-5->LUMO (36%), H-4->L+1 (51%)
11	399.858719038	0.0467	H-5->LUMO (39%), H-4->L+1 (37%)
12	392.877219761	0.0954	H-6->L+1 (14%), H-5->L+1 (73%)
13	388.567735402	0.0354	H-7->LUMO (56%), H-6->LUMO (19%), H-5->LUMO (10%)
14	382.230764288	0.0084	H-7->L+1 (27%), H-6->L+1 (49%), H-5->L+1 (10%)
15	365.767451433	0.0031	H-7->LUMO (29%), H-6->LUMO (57%)
16	359.103843516	0.01	H-7->L+1 (57%), H-6->L+1 (27%)
17	355.520424993	0.0547	H-9->LUMO (23%), H-8->L+1 (27%), HOMO->L+2 (34%)
18	353.321914486	0.1158	H-9->LUMO (49%), H-8->L+1 (29%)
19	347.197404123	0.123	H-8->L+1 (23%), HOMO->L+2 (44%)
20	341.028146694	0.0494	H-12->LUMO (13%), H-8->LUMO (34%), H-1->L+2 (25%)
21	338.837946523	0.019	H-12->LUMO (12%), H-10->L+1 (14%), H-8->LUMO (12%), H-1->L+2 (28%)
22	338.375571115	0.007	H-12->LUMO (13%), H-10->LUMO (11%), H-10->L+1 (44%), H-8->LUMO (10%)
23	337.923665882	0.016	H-12->LUMO (18%), H-10->L+1 (25%), H-8->LUMO (36%)
24	333.371495825	0.004	H-12->LUMO (14%), H-10->LUMO (73%)
25	331.996768007	0.0202	H-3->L+3 (10%), H-3->L+4 (24%), H-1->L+3 (16%), H-1-

			>L+4 (13%)
26	331.827944043	0.0143	H-2->L+3 (10%), H-2->L+4 (13%), H-2->L+5 (19%), HOMO->L+3 (14%), HOMO->L+4 (11%), HOMO->L+5 (11%)
27	330.184269007	0.0128	H-9->L+1 (70%)
28	329.99093211	0.0268	H-13->LUMO (10%), H-12->LUMO (17%), H-11->LUMO (30%), H-9->L+1 (14%)
29	325.982523564	0.0446	H-11->L+1 (69%)
30	325.27269463	0.0054	H-16->LUMO (26%), H-15->LUMO (19%), H-14->LUMO (10%)
31	322.74942864	0.2794	H-16->LUMO (25%), H-13->LUMO (11%), H-1->L+3 (11%)
32	320.596263575	0.0841	H-14->L+1 (59%)
33	318.47163703	0.125	H-13->LUMO (24%), H-13->L+1 (14%), HOMO->L+3 (11%)
34	317.655691661	0.0161	H-12->L+1 (83%)
35	312.893862491	0.0166	HOMO->L+4 (12%), HOMO->L+5 (28%), HOMO->L+7 (14%)
36	312.200521271	0.0396	H-13->L+1 (40%), H-1->L+3 (13%)
37	311.619858276	0.0176	H-18->LUMO (12%), H-17->LUMO (28%)
38	309.534872081	0.0206	H-1->L+4 (13%), HOMO->L+3 (13%)
39	307.729444061	0.0157	H-17->LUMO (11%), H-3->L+2 (10%)
40	305.357222403	0.0487	H-3->L+2 (22%)
41	304.263154954	0.0002	H-14->LUMO (76%)
42	304.076600314	0.0154	H-3->L+2 (11%), H-2->L+2 (53%)
43	303.696737323	0.0097	H-3->L+2 (16%), HOMO->L+7 (22%)
44	303.243635993	0.1252	H-1->L+6 (16%), HOMO->L+4 (22%), HOMO->L+7 (10%)
45	301.84830922	0.1867	H-1->L+4 (15%), HOMO->L+4 (15%), HOMO->L+5 (18%)
46	300.575027303	0.0165	H-18->LUMO (27%), H-15->LUMO (11%), H-1->L+6 (17%)
47	297.752624909	0.008	H-16->L+1 (47%), H-15->L+1 (32%), H-14->L+1 (11%)
48	296.315168998	0.1014	H-18->L+1 (12%), H-16->L+1 (13%)
49	295.137215864	0.0519	H-18->L+1 (14%), H-16->L+1 (11%), H-2->L+7 (28%)
50	293.850148158	0.0053	H-1->L+4 (22%), H-1->L+5 (47%)

Table S6. Selected TD-DFT calculated oscillator strengths and compositions of the major electronic transitions of **5.SO_2**.

No.	Wavelength (nm)	Osc. Strength	Major contribs
1	672.693793132	0.2566	HOMO->LUMO (96%)
2	622.723219549	0.029	H-1->LUMO (36%), HOMO->L+1 (61%)
3	565.363397229	0.0871	H-1->L+1 (94%)
4	532.601026729	1.5143	H-1->LUMO (60%), HOMO->L+1 (35%)
5	461.199244921	0.2632	H-3->LUMO (72%), H-3->L+1 (10%)
6	457.388102749	0.1081	H-3->LUMO (13%), H-2->LUMO (47%), H-2->L+1 (35%)
7	433.05690888	0.0174	H-2->LUMO (41%), H-2->L+1 (53%)
8	419.915305196	0.0068	H-3->LUMO (12%), H-3->L+1 (82%)
9	413.046583643	0.0437	H-4->LUMO (83%)
10	403.017140204	0.0111	H-4->L+1 (76%)
11	398.368386763	0.0473	H-5->LUMO (83%)
12	387.003130793	0.0168	H-5->L+1 (79%)
13	369.473412439	0.3288	H-7->LUMO (11%), H-6->L+1 (12%), HOMO->L+2 (46%), HOMO->L+3 (12%)
14	361.944805174	0.0058	HOMO->L+3 (47%), HOMO->L+4 (29%)
15	361.628096871	0.0046	HOMO->L+2 (19%), HOMO->L+3 (12%), HOMO->L+4 (50%)
16	359.457825038	0.14	H-7->LUMO (12%), H-6->LUMO (38%), H-6->L+1 (14%)
17	353.000008576	0.1709	H-7->LUMO (30%), H-6->L+1 (15%), HOMO->L+2 (10%)
18	349.970906405	0.0123	H-9->LUMO (14%), H-7->LUMO (10%), H-1->L+2 (30%), H-1->L+3 (11%)
19	344.018293597	0.0129	H-10->LUMO (22%), H-9->LUMO (35%), H-8->LUMO (10%), H-1->L+2 (11%)
20	341.244028878	0.0144	H-9->LUMO (20%), H-9->L+1 (13%), H-8->LUMO (29%), H-8->L+1 (24%)
21	337.923665882	0.0085	H-7->LUMO (10%), H-6->LUMO (35%), H-6->L+1 (48%)
22	335.918591705	0.0024	H-1->L+2 (26%), H-1->L+3 (49%), HOMO->L+3 (11%)
23	335.273642543	0.0117	H-10->LUMO (29%), H-7->L+1 (12%)
24	333.156504131	0.0018	H-1->L+4 (76%), HOMO->L+4 (11%)
25	329.789049108	0.0071	H-14->LUMO (20%), H-10->LUMO (20%), H-7->L+1 (18%)
26	327.446104511	0.0417	H-12->LUMO (14%), H-12->L+1 (18%), H-7->L+1 (22%)
27	325.417829428	0.0347	H-14->LUMO (30%), H-8->LUMO (18%), H-8->L+1 (14%), H-7->L+1 (10%)
28	324.073900915	0.0332	H-14->LUMO (19%), H-10->LUMO (13%), H-9->LUMO (12%), H-9->L+1 (15%), H-8->L+1 (16%)
29	323.515794312	0.0018	H-10->L+1 (11%), H-9->L+1 (34%), H-8->L+1 (24%), H-7->L+1 (10%)
30	322.497575789	0.0424	HOMO->L+5 (60%)

31	320.919897014	0.0666	H-1->L+5 (17%), HOMO->L+6 (59%)
32	319.909673372	0.0318	H-13->LUMO (13%), H-11->LUMO (15%), H-10->L+1 (23%)
33	318.963219398	0.0084	H-13->LUMO (29%), H-10->L+1 (23%)
34	317.525528241	0.0095	H-11->LUMO (14%), H-11->L+1 (16%), H-10->L+1 (18%), H-2->L+4 (13%)
35	308.879404614	0.13	H-11->LUMO (14%), H-3->L+2 (14%), H-3->L+3 (19%), H-2->L+4 (21%)
36	307.515732458	0.1417	H-3->L+2 (13%), H-3->L+3 (18%), H-2->L+4 (29%)
37	305.71863645	0.0071	H-12->LUMO (39%), H-12->L+1 (26%), H-11->LUMO (14%), H-11->L+1 (11%)
38	303.577760124	0.0926	H-1->L+5 (56%), HOMO->L+6 (11%)
39	301.708748265	0.044	H-18->LUMO (24%), H-17->LUMO (11%), H-15->LUMO (15%)
40	300.058550368	0.0284	H-18->LUMO (19%), H-17->L+1 (27%)
41	299.399176577	0.0166	H-1->L+6 (65%)
42	299.225758446	0.005	H-17->LUMO (10%), H-16->LUMO (19%), H-13->LUMO (23%)
43	298.41912295	0.0129	H-16->LUMO (10%), H-16->L+1 (11%), H-15->LUMO (32%), H-11->LUMO (12%)
44	296.747787301	0.0028	H-14->LUMO (15%), H-14->L+1 (70%)
45	296.549051669	0.0054	H-16->LUMO (24%), H-15->L+1 (12%), H-13->L+1 (10%), H-11->L+1 (10%)
46	294.450312329	0.0032	H-13->L+1 (10%), HOMO->L+7 (28%), HOMO->L+9 (21%)
47	294.40137012	0.0097	HOMO->L+7 (18%), HOMO->L+8 (59%)
48	293.537082751	0.0475	H-13->L+1 (40%), HOMO->L+9 (11%)
49	291.974832828	0.0848	H-4->L+2 (26%), H-4->L+3 (11%)
50	290.674246289	0.3984	H-13->L+1 (11%), H-1->L+7 (24%), H-1->L+9 (26%)

Table S7. Selected TD-DFT calculated oscillator strengths and compositions of the major electronic transitions of **6**.

No.	Wavelength (nm)	Osc. Strength	Major contribs
1	711.163204154	1.337	HOMO->LUMO (95%)
2	636.012070443	0.39	HOMO->L+1 (95%)
3	593.96470735	0.2049	H-3->LUMO (12%), H-2->L+1 (17%), H-1->LUMO (69%)
4	579.961610124	0.1314	H-3->L+1 (13%), H-2->LUMO (49%), H-1->L+1 (33%)
5	538.92112063	0.2284	H-3->LUMO (16%), H-2->LUMO (17%), H-1->LUMO (11%), H-1->L+1 (43%)
6	537.123393893	0.4736	H-3->LUMO (32%), H-2->L+1 (17%), H-1->LUMO (17%), H-1->L+1 (19%)
7	508.882749188	0.0119	H-3->LUMO (30%), H-2->LUMO (10%), H-2->L+1 (52%)
8	500.824822315	0.0049	H-3->L+1 (73%), H-2->LUMO (14%)
9	450.39302896	0.0067	H-4->LUMO (85%), HOMO->L+2 (13%)
10	432.54323546	0.1314	H-4->L+1 (94%)
11	410.489316025	0.8765	H-4->LUMO (12%), HOMO->L+2 (80%)
12	399.073622416	0.0528	H-6->LUMO (20%), H-6->L+1 (25%), H-5->LUMO (49%)
13	397.831519372	0.2894	H-6->LUMO (43%), H-5->LUMO (13%), H-5->L+1 (36%)
14	376.931848759	0.0025	H-8->L+1 (10%), H-7->LUMO (47%), H-1->L+2 (21%)
15	369.715798456	0.1732	H-10->L+1 (10%), H-8->LUMO (27%), H-7->L+1 (26%)
16	366.188767831	0.0072	H-1->L+2 (58%)
17	363.185286227	0.0021	H-8->LUMO (12%), H-6->LUMO (22%), H-5->LUMO (13%), H-5->L+1 (41%)
18	359.885614386	0.0097	H-6->L+1 (54%), H-5->LUMO (17%)
19	353.896766034	0.0545	H-11->LUMO (15%), H-10->LUMO (15%), H-10->L+1 (13%), HOMO->L+3 (24%)
20	350.753063857	0.0412	H-11->LUMO (14%), H-9->LUMO (10%), H-8->LUMO (24%), H-2->L+2 (26%)
21	349.931396269	0.1672	H-2->L+2 (60%)
22	347.850049132	0.017	H-3->L+2 (74%)
23	347.314115671	0.0184	H-9->LUMO (23%), H-7->L+1 (37%)
24	343.894247392	0.0069	H-9->LUMO (18%), H-8->L+1 (33%), H-7->LUMO (20%)
25	342.110297763	0.01	H-9->LUMO (40%), H-8->L+1 (12%), H-7->L+1 (21%)

26	339.004711159	0.008	H-12->LUMO (49%), H-12->L+1 (40%)
27	337.096772736	0.0206	H-13->LUMO (16%), H-8->L+1 (13%), HOMO->L+3 (17%)
28	336.100715694	0.0292	H-13->LUMO (49%), H-13->L+1 (18%)
29	333.120699138	0.0038	H-9->L+1 (85%)
30	330.589251846	0.0082	H-2->L+4 (20%), H-1->L+5 (14%), HOMO->L+4 (24%)
31	329.272303108	0.0015	H-2->L+5 (17%), H-1->L+4 (14%), HOMO->L+5 (19%)
32	326.566383112	0.0664	H-17->LUMO (27%), H-17->L+1 (26%), H-15->LUMO (14%)
33	325.742717178	0.0129	H-16->LUMO (27%), H-15->LUMO (14%), HOMO->L+3 (11%)
34	324.787009515	0.0093	H-15->LUMO (13%), H-14->LUMO (21%), H-14->L+1 (17%)
35	323.777695694	0.0058	H-18->LUMO (36%), H-18->L+1 (16%)
36	319.431630371	0.0369	H-16->L+1 (14%), H-10->LUMO (16%), H-10->L+1 (16%), H-4->L+2 (26%)
37	318.545277766	0.0168	H-10->LUMO (26%), H-10->L+1 (27%), H-4->L+2 (16%)
38	317.574327021	0.011	H-16->LUMO (23%), HOMO->L+5 (11%)
39	316.02822444	0.0106	H-2->L+4 (11%), HOMO->L+4 (47%)
40	315.008493641	0.005	HOMO->L+5 (35%)
41	314.234065826	0.0015	H-11->LUMO (26%), H-11->L+1 (66%)
42	313.115117338	0.0941	H-16->L+1 (17%), H-15->L+1 (13%), H-4->L+2 (11%), H-1->L+3 (35%)
43	312.578326011	0.026	H-20->LUMO (26%), H-20->L+1 (16%), H-19->LUMO (19%)
44	311.21311532	0.0119	H-20->LUMO (11%), H-19->LUMO (11%), H-19->L+1 (14%), H-12->LUMO (22%), H-12->L+1 (24%)
45	310.908754231	0.0101	H-19->L+1 (11%), H-12->LUMO (23%), H-12->L+1 (30%)
46	307.309934347	0.0003	H-13->LUMO (25%), H-13->L+1 (71%)
47	306.406170948	0.1466	HOMO->L+6 (59%)
48	305.146791889	0.0249	HOMO->L+7 (53%)
49	304.382670101	0.1651	H-15->L+1 (16%), H-14->LUMO (10%), H-1->L+3 (35%)
50	301.005566915	0.0057	H-15->L+1 (10%), H-14->LUMO (31%), H-14->L+1 (44%)

Table S8. Selected TD-DFT calculated oscillator strengths and compositions of the major electronic transitions of **6.SO_2**.

No.	Wavelength (nm)	Osc. Strength	Major contribs
1	701.387073668	1.2006	HOMO->LUMO (98%)
2	630.09703213	0.2882	HOMO->L+1 (94%)
3	552.588104525	0.9429	H-1->LUMO (94%)
4	537.51926217	0.1875	H-1->L+1 (94%)
5	460.343047608	0.3281	H-4->LUMO (51%), H-3->LUMO (12%), H-3->L+1 (34%)
6	459.762646984	0.0228	H-4->LUMO (13%), H-4->L+1 (31%), H-3->LUMO (52%)
7	452.530086182	0.0115	H-2->LUMO (84%), HOMO->L+2 (11%)
8	435.398907895	0.1374	H-2->L+1 (90%)
9	415.663782393	0.0033	H-4->LUMO (11%), H-4->L+1 (14%), H-3->LUMO (23%), H-3->L+1 (48%)
10	414.136525527	0.0012	H-4->LUMO (20%), H-4->L+1 (49%), H-3->LUMO (12%), H-3->L+1 (16%)
11	407.0661009	0.8481	HOMO->L+2 (81%)
12	378.312003821	0.0052	H-6->L+1 (12%), H-5->LUMO (58%), H-1->L+2 (13%)
13	371.766695689	0.1749	H-9->LUMO (10%), H-8->L+1 (12%), H-6->LUMO (32%), H-5->L+1 (28%)
14	371.0768377	0.0018	H-1->L+3 (10%), HOMO->L+3 (87%)
15	370.500218181	0.0024	H-1->L+4 (10%), HOMO->L+4 (87%)
16	364.573609187	0.0167	H-9->L+1 (10%), H-8->LUMO (16%), H-1->L+2 (55%)
17	354.189952899	0.06	H-8->LUMO (17%), H-1->L+2 (15%), HOMO->L+5 (30%)
18	352.54831953	0.0446	H-7->LUMO (23%), H-6->LUMO (51%), H-5->L+1 (10%)
19	349.862274994	0.1607	H-9->LUMO (21%), H-8->L+1 (10%), H-5->L+1 (46%)
20	346.566577253	0.0017	H-12->LUMO (10%), H-6->L+1 (57%), H-5->LUMO (20%)
21	344.697358871	0.0328	H-7->LUMO (67%)
22	341.751958467	0.0097	H-10->LUMO (58%), H-10->L+1 (35%)
23	338.255560136	0.0506	H-11->LUMO (51%), H-11->L+1 (26%)
24	336.191851764	0.0036	H-7->L+1 (60%), HOMO->L+5 (11%)
25	333.138600672	0.0095	H-7->L+1 (25%), H-1->L+4 (12%), HOMO->L+5 (16%)
26	332.334931815	0.0049	H-1->L+3 (25%), H-1->L+4 (50%)
27	331.890122366	0.0009	H-1->L+3 (55%), H-1->L+4 (19%), HOMO->L+3 (10%)
28	329.48230936	0.0102	H-15->LUMO (11%), H-12->LUMO (32%), HOMO->L+5 (13%), HOMO->L+7 (12%)
29	328.748456839	0.0396	H-16->LUMO (23%), H-16->L+1 (16%), H-15->LUMO (13%), HOMO->L+6 (10%)

30	326.394442722	0.0805	HOMO->L+6 (62%)
31	325.631498391	0.0219	H-16->LUMO (21%), H-16->L+1 (12%), H-12->LUMO (18%)
32	322.522743385	0.0003	H-13->LUMO (16%), H-12->L+1 (22%), H-2->L+2 (27%)
33	320.107903057	0.0075	H-14->LUMO (26%), H-13->L+1 (17%), HOMO->L+7 (13%)
34	319.530418567	0.0254	H-14->L+1 (13%), H-13->LUMO (13%), H-8->LUMO (15%), H-8->L+1 (24%)
35	318.528910215	0.0156	H-8->LUMO (20%), H-8->L+1 (20%), H-2->L+2 (11%)
36	317.916338912	0.0118	H-8->L+1 (10%), HOMO->L+7 (39%)
37	316.957315265	0.0028	H-9->LUMO (28%), H-9->L+1 (57%)
38	313.083490347	0.1255	H-12->L+1 (37%), H-2->L+2 (21%), H-1->L+5 (31%)
39	312.121926874	0.0002	H-10->LUMO (37%), H-10->L+1 (62%)
40	309.61990064	0.0004	H-11->LUMO (34%), H-11->L+1 (65%)
41	309.326363485	0.2996	H-4->L+3 (10%), H-3->L+4 (15%), H-1->L+5 (13%)
42	307.188109839	0.0655	H-14->LUMO (12%), H-4->L+3 (27%), H-3->L+4 (24%)
43	304.884161246	0.0703	H-12->L+1 (13%), H-1->L+5 (30%)
44	302.039496729	0.0123	H-3->L+2 (29%), HOMO->L+9 (11%)
45	301.840960688	0.0097	H-3->L+2 (18%), HOMO->L+8 (32%)
46	300.881386687	0.0222	H-3->L+2 (33%), HOMO->L+9 (34%)
47	300.443921323	0.075	H-4->L+2 (47%), HOMO->L+8 (24%)
48	299.529372146	0.0186	H-17->LUMO (14%), H-4->L+2 (15%), HOMO->L+8 (10%), HOMO->L+9 (23%)
49	299.110257924	0.0017	H-20->LUMO (33%), H-19->L+1 (14%)
50	298.577225797	0.0057	H-19->LUMO (17%), H-18->LUMO (13%), H-17->LUMO (23%), H-17->L+1 (11%)

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

Sum of imaginary frequencies= 0

Total Energy (Hartree) = -1844.165802

Atom	X	Y	Z	Atom	X	Y	Z
C	-0.940610000	-0.794816000	1.500321000	C	-0.549016000	0.180850000	0.572343000
C	-1.553731000	0.850131000	-0.149482000	C	-2.898051000	0.570143000	0.066432000
C	-3.292139000	-0.418518000	0.995813000	C	-2.284720000	-1.099020000	1.699911000
S	-4.145224000	1.537608000	-0.761732000	C	-5.397088000	0.276250000	-0.920498000
C	-5.543363000	-0.684212000	0.100442000	N	-4.655753000	-0.688538000	1.203406000
C	-6.259439000	0.287427000	-2.016912000	C	-7.308318000	-0.631482000	-2.099551000
C	-7.463555000	-1.583059000	-1.092970000	C	-6.580375000	-1.623111000	-0.011724000
C	-5.031016000	-1.464152000	2.379169000	C	0.872074000	0.507328000	0.357696000
C	1.807840000	-0.510467000	0.155312000	C	1.294007000	1.858528000	0.359423000
C	1.613081000	-1.917373000	0.062762000	C	2.844976000	-2.492612000	-0.141078000
C	3.807091000	-1.440816000	-0.201392000	N	3.171897000	-0.249965000	-0.027433000
C	0.585340000	3.061731000	0.566435000	C	1.511224000	4.105387000	0.479784000
C	2.760384000	3.519110000	0.240216000	N	2.631835000	2.176054000	0.168254000
B	3.798681000	1.176774000	0.043742000	F	4.666909000	1.274533000	1.122380000
F	4.513654000	1.457787000	-1.146413000	C	5.206954000	-1.654337000	-0.415873000
C	5.901518000	-2.868345000	-0.328259000	C	7.255047000	-2.608799000	-0.614629000
C	7.360357000	-1.247865000	-0.881249000	N	6.130046000	-0.686396000	-0.751148000
H	-0.184068000	-1.310606000	2.080769000	H	-1.274243000	1.593943000	-0.887489000
H	-2.548204000	-1.868366000	2.415089000	H	-6.114804000	1.028490000	-2.797302000
H	-7.988169000	-0.604010000	-2.944978000	H	-8.265435000	-2.312934000	-1.148045000
H	-6.700867000	-2.390617000	0.743293000	H	-4.454954000	-1.108014000	3.235916000
H	-4.853769000	-2.543142000	2.256568000	H	-6.091902000	-1.303266000	2.581331000
H	0.655130000	-2.411809000	0.121200000	H	3.072641000	-3.539606000	-0.279096000
H	-0.473799000	3.135634000	0.763503000	H	1.317275000	5.163893000	0.583337000
H	3.731152000	3.981658000	0.128663000	H	5.461260000	-3.817588000	-0.057240000
H	8.067926000	-3.321237000	-0.624428000	H	8.216567000	-0.649371000	-1.156576000
H	5.876384000	0.275001000	-0.955424000				

Table S10. S_0 optimized geometry of compound **3.SO$_2$** at B3LYP/6-31g (d,p) level of theory

Sum of imaginary frequencies= 0

Total Energy (Hartree) = -1994.558630

Atom	X	Y	Z	Atom	X	Y	Z
F	-4.923969000	1.563189000	0.758788000	F	-4.923969000	1.563189000	0.758788000
F	-4.838887000	1.061085000	-1.468268000	F	-4.838887000	1.061085000	-1.468268000
B	-4.074396000	1.209227000	-0.284509000	B	-4.074396000	1.209227000	-0.284509000
N	-6.198269000	-1.069382000	-0.482367000	N	-6.198269000	-1.069382000	-0.482367000
C	-7.369524000	-1.754237000	-0.426032000	C	-7.369524000	-1.754237000	-0.426032000
C	-7.176313000	-2.896623000	0.343897000	C	-7.176313000	-2.896623000	0.343897000
C	-5.830471000	-2.896639000	0.751699000	C	-5.830471000	-2.896639000	0.751699000
C	-5.224126000	-1.743247000	0.229132000	C	-5.224126000	-1.743247000	0.229132000
N	-3.322607000	-0.115713000	0.057438000	N	-3.322607000	-0.115713000	0.057438000
C	-3.858866000	-1.330686000	0.374952000	C	-3.858866000	-1.330686000	0.374952000
C	-2.825863000	-2.171393000	0.891396000	C	-2.825863000	-2.171393000	0.891396000
C	-1.657576000	-1.450441000	0.884439000	C	-1.657576000	-1.450441000	0.884439000
N	-3.005312000	2.290589000	-0.532523000	N	-3.005312000	2.290589000	-0.532523000
C	-3.232737000	3.527682000	-1.032599000	C	-3.232737000	3.527682000	-1.032599000
C	-2.025719000	4.228166000	-1.139282000	C	-2.025719000	4.228166000	-1.139282000
C	-1.018427000	3.370453000	-0.688473000	C	-1.018427000	3.370453000	-0.688473000
C	-1.950545000	-0.160123000	0.354476000	C	-1.950545000	-0.160123000	0.354476000
C	-1.640781000	2.161896000	-0.305154000	C	-1.640781000	2.161896000	-0.305154000
C	-1.108196000	0.937376000	0.167168000	C	-1.108196000	0.937376000	0.167168000
C	5.097874000	1.408863000	2.301411000	C	5.097874000	1.408863000	2.301411000
C	6.712360000	0.531852000	0.107139000	C	6.712360000	0.531852000	0.107139000
C	7.544149000	0.012318000	-0.879620000	C	7.544149000	0.012318000	-0.879620000
C	7.093709000	-0.967385000	-1.770610000	C	7.093709000	-0.967385000	-1.770610000
C	5.793579000	-1.441196000	-1.648752000	C	5.793579000	-1.441196000	-1.648752000
N	4.522913000	0.620690000	1.207242000	N	4.522913000	0.620690000	1.207242000
C	5.389678000	0.068178000	0.249572000	C	5.389678000	0.068178000	0.249572000
C	4.965073000	-0.940156000	-0.641721000	C	4.965073000	-0.940156000	-0.641721000
S	3.382904000	-1.684262000	-0.386682000	S	3.382904000	-1.684262000	-0.386682000

Table S11. S_0 optimized geometry of compound **4** at B3LYP/6-31g (d,p) level of theory
Sum of imaginary frequencies= 0
Total Energy (Hartree) = -1957.494400

Atom	X	Y	Z	Atom	X	Y	Z
C	-1.470580000	-0.787465000	1.523436000	C	-1.070324000	0.194633000	0.604960000
C	-2.066146000	0.847654000	-0.144644000	C	-3.410738000	0.546387000	0.034939000
C	-3.813705000	-0.447362000	0.956397000	C	-2.813995000	-1.110448000	1.689116000
S	-4.648799000	1.496731000	-0.824814000	C	-5.882264000	0.221059000	-1.009813000
C	-6.039740000	-0.741500000	0.006971000	N	-5.175211000	-0.739418000	1.129076000
C	-6.720606000	0.223283000	-2.124795000	C	-7.756567000	-0.707624000	-2.230560000
C	-7.922515000	-1.661882000	-1.228203000	C	-7.062823000	-1.692400000	-0.128020000
C	-5.570049000	-1.517193000	2.297767000	C	0.348375000	0.545996000	0.432792000
C	1.312857000	-0.462339000	0.271007000	C	0.746073000	1.899181000	0.433681000
C	1.144949000	-1.869519000	0.185796000	C	2.397341000	-2.425138000	0.029423000
C	3.334175000	-1.358277000	-0.009500000	N	2.672824000	-0.176648000	0.131580000
C	0.009790000	3.094021000	0.614136000	C	0.916872000	4.150776000	0.546832000
C	2.185187000	3.583796000	0.346842000	N	2.084247000	2.241254000	0.279178000
B	3.273293000	1.262442000	0.195034000	F	4.114119000	1.391718000	1.289010000
F	4.005424000	1.536007000	-0.985632000	C	4.751519000	-1.539428000	-0.175998000
C	5.472792000	-2.739971000	-0.021712000	C	6.816683000	-2.463486000	-0.285585000
C	6.905482000	-1.103397000	-0.606544000	N	5.644197000	-0.568770000	-0.526421000
H	-0.722471000	-1.290152000	2.125667000	H	-1.778930000	1.593578000	-0.877497000
H	-3.084029000	-1.882042000	2.399193000	H	-6.567762000	0.966600000	-2.901418000
H	-8.418188000	-0.687285000	-3.090471000	H	-8.714259000	-2.401105000	-1.301156000
H	-7.190735000	-2.462174000	0.623414000	H	-5.019561000	-1.152483000	3.167552000
H	-5.377282000	-2.593930000	2.181214000	H	-6.637155000	-1.367843000	2.473608000
H	0.195446000	-2.381982000	0.216264000	H	2.648112000	-3.469199000	-0.089055000
H	-1.055223000	3.149907000	0.782965000	H	0.702985000	5.206278000	0.639252000
H	3.149758000	4.064934000	0.262310000	H	5.043140000	-3.685934000	0.275878000
H	7.656046000	-3.142737000	-0.251854000	H	5.372536000	0.381384000	-0.767645000
C	8.053111000	-0.296730000	-0.973306000	H	7.821725000	0.772807000	-1.173303000
O	9.195116000	-0.727341000	-1.063733000				

Table S12. S_0 optimized geometry of compound **4.SO_2** at B3LYP/6-31g (d,p) level of theory

Sum of imaginary frequencies= 0

Total Energy (Hartree) = -2107.887924

Atom	X	Y	Z	Atom	X	Y	Z
F	-4.381733000	1.826583000	0.859845000	F	-4.335443000	1.251127000	-1.351027000
B	-3.557329000	1.416982000	-0.179510000	N	-5.734945000	-0.808051000	-0.286548000
C	-6.949058000	-1.441807000	-0.179015000	C	-6.781923000	-2.540933000	0.674142000
C	-5.443502000	-2.561713000	1.070599000	C	-4.798818000	-1.465358000	0.460417000
N	-2.838885000	0.081382000	0.194657000	C	-3.407159000	-1.103486000	0.566515000
C	-2.399729000	-1.961527000	1.084346000	C	-1.203232000	-1.280784000	1.024647000
N	-2.457927000	2.458433000	-0.472192000	C	-2.653605000	3.685869000	-0.998017000
C	-1.423844000	4.343808000	-1.154209000	C	-0.437695000	3.466697000	-0.707804000
C	-1.467067000	-0.003695000	0.460255000	C	-1.091413000	2.287120000	-0.274180000
C	-0.588840000	1.064503000	0.215726000	C	5.689031000	1.370545000	2.150157000
C	7.202044000	0.327996000	-0.043339000	C	7.984093000	-0.270337000	-1.026177000
C	7.468902000	-1.268505000	-1.859562000	C	6.153882000	-1.679946000	-1.683324000
N	5.049872000	0.561217000	1.107584000	C	5.865745000	-0.071578000	0.153741000
C	5.374913000	-1.099025000	-0.679623000	S	3.770249000	-1.761769000	-0.352386000
C	2.930187000	1.733811000	1.474338000	C	3.669416000	0.659907000	0.933800000
C	2.945287000	-0.286894000	0.175954000	C	1.580166000	-0.162787000	-0.067626000
C	0.861165000	0.911882000	0.465349000	C	1.567917000	1.849970000	1.244158000
H	-5.523615000	0.004454000	-0.862593000	H	-7.564832000	-3.228182000	0.959262000
H	-4.975899000	-3.268461000	1.740486000	H	-2.560881000	-2.969748000	1.435773000
H	-0.236499000	-1.637010000	1.346771000	H	-3.648321000	4.030785000	-1.243241000
H	-1.285753000	5.336653000	-1.557206000	H	0.629754000	3.630039000	-0.705944000
H	6.613929000	0.884049000	2.458157000	H	5.912369000	2.389921000	1.815306000
H	5.033064000	1.414364000	3.019038000	H	7.624582000	1.129943000	0.547691000
H	9.007506000	0.067259000	-1.155635000	H	8.084530000	-1.716897000	-2.631317000
H	5.716453000	-2.453017000	-2.305847000	H	3.425432000	2.500775000	2.055042000
H	1.091667000	-0.903903000	-0.690198000	H	1.034883000	2.687566000	1.680289000
O	3.852894000	-2.691196000	0.795923000	O	3.159091000	-2.268796000	-1.596847000
C	-8.127870000	-0.966758000	-0.876135000	H	-7.972208000	-0.057686000	-1.493854000
O	-9.228197000	-1.503711000	-0.810443000				

Table S13. S_0 optimized geometry of compound **5** at B3LYP/6-31g (d,p) level of theory
Sum of imaginary frequencies= 0
Total Energy (Hartree) = -3874.015623

Atom	X	Y	Z	Atom	X	Y	Z
N	-1.355681000	7.368729000	-0.212895000	C	-1.769090000	7.308542000	1.010934000
F	-1.399821000	2.843721000	0.080294000	F	-3.164953000	3.481207000	-1.214752000
B	-2.639124000	2.443866000	-0.412691000	N	-2.874953000	5.064764000	1.125186000
C	-2.465933000	6.241899000	1.695818000	C	-2.789105000	6.178647000	3.060438000
C	-3.400328000	4.941882000	3.294472000	C	-3.437123000	4.251380000	2.070437000
N	-3.633235000	2.143037000	0.749030000	C	-3.920067000	2.922166000	1.828876000
C	-4.773253000	2.199949000	2.708535000	C	-5.011448000	0.969118000	2.136731000
N	-2.509241000	1.158338000	-1.252405000	C	-1.738942000	1.012700000	-2.349850000
C	-2.022274000	-0.214155000	-2.969228000	C	-3.005884000	-0.839912000	-2.200181000
C	-4.307865000	0.929827000	0.901521000	C	-3.296078000	0.020485000	-1.117757000
C	-4.183615000	-0.114043000	-0.026322000	C	-6.480905000	-6.169861000	0.882289000
C	-9.053512000	-6.144462000	-0.348834000	C	-10.379661000	-6.194244000	-0.783963000
C	-11.200170000	-5.071802000	-0.685390000	C	-10.684199000	-3.892150000	-0.143746000
N	-7.199522000	-4.914297000	0.700868000	C	-8.533224000	-4.976014000	0.228374000
C	-9.371812000	-3.847735000	0.326953000	S	-8.768066000	-2.376875000	1.136279000
C	-5.077880000	-3.784382000	0.195291000	C	-6.448362000	-3.743713000	0.505778000
C	-7.062504000	-2.476978000	0.628675000	C	-6.332253000	-1.310252000	0.435460000
C	-4.955791000	-1.354941000	0.147844000	C	-4.345383000	-2.612760000	0.030211000
N	-1.718672000	6.352962000	-1.051601000	C	-0.869056000	5.430000000	-1.347125000
F	1.542009000	1.679964000	-2.736001000	F	0.768165000	1.285883000	-0.636194000
B	1.854033000	1.096615000	-1.504608000	N	1.086905000	4.031796000	-0.973495000
C	0.490949000	5.261900000	-0.882085000	C	1.456477000	6.177263000	-0.443237000
C	2.652525000	5.469229000	-0.282681000	C	2.402935000	4.120768000	-0.599005000
N	3.144773000	1.745543000	-0.907136000	C	3.353141000	3.049386000	-0.573053000
C	4.722456000	3.222886000	-0.214732000	C	5.346164000	2.005982000	-0.353798000
N	2.137993000	-0.411923000	-1.652426000	C	1.221022000	-1.357491000	-1.952146000
C	1.830789000	-2.619371000	-1.977352000	C	3.178152000	-2.424990000	-1.664209000
C	4.361699000	1.067308000	-0.771323000	C	3.362312000	-1.038562000	-1.466693000
C	4.490670000	-0.299232000	-1.042890000	C	10.158443000	-3.517115000	-1.575246000
C	10.606895000	-4.604284000	1.023005000	C	10.996165000	-5.048708000	2.288519000
C	10.672436000	-4.313818000	3.427858000	C	9.954620000	-3.122983000	3.293578000
N	9.537203000	-2.909870000	-0.404489000	C	9.915541000	-3.392417000	0.871705000
C	9.595946000	-2.654912000	2.029373000	S	8.796054000	-1.068738000	1.862693000
C	7.502664000	-2.485762000	-1.714834000	C	8.287469000	-2.287600000	-0.566113000
C	7.787178000	-1.429302000	0.438013000	C	6.552759000	-0.806321000	0.292629000
C	5.785087000	-0.981566000	-0.872648000	C	6.280769000	-1.837021000	-1.868013000
H	-1.532385000	8.173118000	1.628433000	H	-2.851467000	4.866100000	0.131536000
H	-2.574146000	6.952437000	3.784551000	H	-3.745038000	4.548525000	4.240233000
H	-5.160213000	2.583256000	3.641713000	H	-5.607638000	0.161751000	2.534690000

H	-1.014162000	1.762545000	-2.631000000	H	-1.556948000	-0.585828000	-3.871481000
H	-3.478207000	-1.793944000	-2.380890000	H	-7.151881000	-6.893790000	1.349024000
H	-6.108034000	-6.590817000	-0.063299000	H	-5.634113000	-5.998757000	1.550214000
H	-8.424098000	-7.018481000	-0.464090000	H	-10.760688000	-7.115063000	-1.214822000
H	-12.228433000	-5.105666000	-1.030588000	H	-11.303823000	-3.003513000	-0.069816000
H	-4.575356000	-4.737245000	0.084280000	H	-6.831459000	-0.349855000	0.502330000
H	-3.283448000	-2.670248000	-0.179354000	H	-1.253134000	4.659750000	-2.009932000
H	0.573212000	3.158282000	-1.032723000	H	1.284285000	7.233338000	-0.302599000
H	3.610492000	5.871048000	0.014903000	H	5.164478000	4.159038000	0.093024000
H	6.388744000	1.779069000	-0.190038000	H	0.187731000	-1.084328000	-2.114592000
H	1.334475000	-3.557426000	-2.184322000	H	3.947852000	-3.174990000	-1.557251000
H	11.224703000	-3.646224000	-1.378643000	H	9.725084000	-4.495212000	-1.832180000
H	10.039457000	-2.844490000	-2.427334000	H	10.840482000	-5.206671000	0.153484000
H	11.542129000	-5.983029000	2.376348000	H	10.966609000	-4.661514000	4.412879000
H	9.682435000	-2.542942000	4.170257000	H	7.847298000	-3.149558000	-2.498034000
H	6.173002000	-0.180676000	1.092717000	H	5.704977000	-1.985833000	-2.774419000

Table S14. S_0 optimized geometry of compound **5.SO$_2$** at B3LYP/6-31g (d,p) level of theory

Sum of imaginary frequencies= 0

Total Energy (Hartree) = -4174.807988

Atom	X	Y	Z	Atom	X	Y	Z
N	-1.167481000	7.078262000	-0.135323000	C	-1.908063000	7.219648000	0.918944000
F	-1.738437000	2.329515000	1.255713000	F	-2.621881000	3.001473000	-0.743554000
B	-2.718317000	2.062129000	0.308921000	N	-3.169835000	5.055889000	1.047987000
C	-2.877434000	6.320170000	1.497380000	C	-3.680240000	6.558829000	2.625561000
C	-4.469364000	5.424959000	2.832409000	C	-4.132677000	4.485278000	1.839059000
N	-4.139042000	2.137240000	0.953335000	C	-4.679421000	3.164586000	1.672424000
C	-5.899401000	2.726733000	2.261544000	C	-6.097000000	1.417472000	1.885481000
N	-2.551696000	0.641276000	-0.274404000	C	-1.496344000	0.200263000	-0.994770000
C	-1.727216000	-1.114832000	-1.424835000	C	-2.983367000	-1.483929000	-0.946045000
C	-5.001868000	1.040551000	1.058920000	C	-3.492296000	-0.382690000	-0.216645000
C	-4.713545000	-0.196927000	0.466833000	C	-8.052129000	-5.762760000	1.538293000
C	-10.015169000	-5.873383000	-0.541721000	C	-11.061047000	-5.929223000	-1.457428000
C	-11.626144000	-4.765640000	-1.989572000	C	-11.141240000	-3.531617000	-1.575170000
N	-8.415857000	-4.563809000	0.776715000	C	-9.505791000	-4.633876000	-0.107328000
C	-10.109111000	-3.472770000	-0.635557000	S	-9.634409000	-1.900326000	0.015612000
C	-6.171860000	-3.642808000	1.123831000	C	-7.523374000	-3.491059000	0.747920000
C	-7.915350000	-2.208708000	0.305006000	C	-7.019346000	-1.147474000	0.201752000
C	-5.680104000	-1.313583000	0.568183000	C	-5.283048000	-2.582016000	1.035956000
N	-1.417434000	5.985963000	-0.922571000	C	-0.451543000	5.171244000	-1.196031000
F	3.028004000	2.579776000	-3.383463000	F	1.660813000	1.487688000	-1.917832000
B	2.999153000	1.614424000	-2.384809000	N	1.672702000	4.035071000	-0.990457000
C	0.898791000	5.127780000	-0.690051000	C	1.680594000	5.989150000	0.099021000
C	2.930076000	5.385036000	0.265488000	C	2.908297000	4.149098000	-0.412391000
N	3.953585000	2.014137000	-1.216267000	C	3.944436000	3.156604000	-0.464916000
C	5.143985000	3.217478000	0.301417000	C	5.885811000	2.098696000	0.004598000
N	3.460124000	0.243026000	-2.908305000	C	2.796622000	-0.527168000	-3.800289000
C	3.504328000	-1.715112000	-4.025297000	C	4.647350000	-1.662922000	-3.225625000
C	5.145853000	1.330564000	-0.937999000	C	4.616869000	-0.430470000	-2.533130000
C	5.480709000	0.122354000	-1.560656000	C	11.345902000	-2.837007000	-1.231532000
C	11.130435000	-4.693640000	0.934540000	C	11.125938000	-5.533087000	2.043985000
C	10.318337000	-5.267914000	3.154802000	C	9.521769000	-4.129846000	3.151522000
N	10.285661000	-2.706874000	-0.227293000	C	10.330238000	-3.534540000	0.907347000
C	9.544767000	-3.271297000	2.049700000	S	8.669869000	-1.738900000	2.141637000
C	8.818193000	-1.659489000	-1.886951000	C	9.141171000	-1.976093000	-0.550315000
C	8.226683000	-1.550536000	0.437956000	C	7.044402000	-0.884048000	0.125006000
C	6.731965000	-0.583806000	-1.204311000	C	7.648014000	-0.983370000	-2.197577000
H	-1.766766000	8.151902000	1.462445000	H	-2.787865000	4.638278000	0.203946000
H	-3.669421000	7.464243000	3.216036000	H	-5.183025000	5.266608000	3.627728000
H	-6.548336000	3.337862000	2.871253000	H	-6.921667000	0.778302000	2.162627000

H	-0.632811000	0.826454000	-1.172510000	H	-1.050027000	-1.711386000	-2.019013000
H	-3.492798000	-2.423021000	-1.103421000	H	-8.962145000	-6.283927000	1.834020000
H	-7.414006000	-6.447943000	0.968449000	H	-7.532472000	-5.462411000	2.447681000
H	-9.574108000	-6.797278000	-0.191069000	H	-11.424107000	-6.901235000	-1.776157000
H	-12.431321000	-4.822904000	-2.713522000	H	-11.553636000	-2.605284000	-1.960388000
H	-5.803067000	-4.602500000	1.461163000	H	-7.376387000	-0.197637000	-0.180362000
H	-4.253540000	-2.737854000	1.338792000	H	-0.729451000	4.364161000	-1.871362000
H	1.349179000	3.195003000	-1.462043000	H	1.354120000	6.940988000	0.486078000
H	3.772485000	5.787555000	0.808943000	H	5.398138000	4.004386000	0.995792000
H	6.855083000	1.837369000	0.401601000	H	1.857777000	-0.199094000	-4.223775000
H	3.203308000	-2.514225000	-4.687324000	H	5.410515000	-2.420563000	-3.126526000
H	12.293852000	-3.013615000	-0.724168000	H	11.159440000	-3.652665000	-1.939600000
H	11.433792000	-1.899495000	-1.779724000	H	11.733221000	-4.960552000	0.076280000
H	11.748898000	-6.421825000	2.028271000	H	10.313112000	-5.937829000	4.007374000
H	8.883466000	-3.885714000	3.993866000	H	9.469604000	-1.967507000	-2.694164000
H	6.366627000	-0.617538000	0.928233000	H	7.436308000	-0.757192000	-3.236856000
O	-10.302294000	-1.693396000	1.319756000	O	-9.798279000	-0.849098000	-1.007927000
O	7.456819000	-1.888359000	2.969688000	O	9.615836000	-0.660585000	2.504832000

Table S15. S_0 optimized geometry of compound **6** at B3LYP/6-31g (d,p) level of theory
Sum of imaginary frequencies= 0
Total Energy (Hartree) = -4105.108211

Atom	X	Y	Z	Atom	X	Y	Z
N	-3.177785000	3.829798000	0.094103000	C	-3.967105000	4.849922000	0.104938000
F	-6.333638000	1.164016000	2.227361000	F	-5.667001000	0.745633000	0.082643000
B	-6.697713000	0.568425000	1.029260000	N	-5.981416000	3.449927000	0.200259000
C	-5.393038000	4.682685000	0.166341000	C	-6.411297000	5.646456000	0.196432000
C	-7.629864000	4.961285000	0.240885000	C	-7.342646000	3.582740000	0.246701000
N	-8.032699000	1.193309000	0.507448000	C	-8.294111000	2.510240000	0.280199000
C	-9.693043000	2.680219000	0.082367000	C	-10.281334000	1.440692000	0.199684000
N	-6.951144000	-0.944995000	1.199981000	C	-6.006672000	-1.869271000	1.469779000
C	-6.583761000	-3.147477000	1.503101000	C	-7.942427000	-2.983188000	1.229364000
C	-9.245875000	0.501128000	0.457918000	C	-8.166521000	-1.598731000	1.048192000
C	-9.330333000	-0.877851000	0.700329000	C	-14.597460000	-4.720649000	1.187261000
C	-16.749668000	-3.083346000	0.271116000	C	-17.841084000	-2.428936000	-0.304613000
C	-17.660414000	-1.566893000	-1.384853000	C	-16.374190000	-1.362646000	-1.890453000
N	-14.342915000	-3.591466000	0.300743000	C	-15.458024000	-2.913563000	-0.249618000
C	-15.285554000	-2.041587000	-1.343129000	S	-13.668928000	-1.871884000	-2.080234000
C	-12.262893000	-3.121063000	1.516570000	C	-13.113790000	-2.924096000	0.415004000
C	-12.691234000	-2.033133000	-0.598098000	C	-11.481694000	-1.357771000	-0.491909000
C	-10.621033000	-1.577030000	0.599468000	C	-11.031908000	-2.477836000	1.594373000
N	2.406908000	4.377871000	-0.306715000	C	3.189028000	3.353152000	-0.316128000
F	6.256389000	0.204995000	-2.359918000	F	5.627653000	-0.301285000	-0.224744000
B	6.704713000	-0.295425000	-1.146888000	N	5.441724000	2.402549000	-0.376134000
C	4.619501000	3.497467000	-0.362039000	C	5.432069000	4.641284000	-0.394946000
C	6.759084000	4.207999000	-0.418673000	C	6.751994000	2.798769000	-0.407132000
N	7.880917000	0.577988000	-0.606049000	C	7.887376000	1.926300000	-0.405821000
C	9.225403000	2.358189000	-0.185306000	C	10.036114000	1.247928000	-0.257112000
N	7.238032000	-1.734734000	-1.281442000	C	6.489914000	-2.823493000	-1.560077000
C	7.292809000	-3.972156000	-1.541591000	C	8.587590000	-3.554063000	-1.226577000
C	9.200918000	0.125252000	-0.511789000	C	8.546616000	-2.149897000	-1.073570000
C	9.546770000	-1.218069000	-0.712575000	C	15.443385000	-4.042910000	-0.900611000
C	17.224963000	-2.012258000	0.020887000	C	18.157053000	-1.152323000	0.606197000
C	17.782294000	-0.305400000	1.647792000	C	16.462301000	-0.324447000	2.104892000
N	14.953423000	-2.952034000	-0.066854000	C	15.905141000	-2.065329000	0.493790000
C	15.536351000	-1.207054000	1.548770000	S	13.889264000	-1.313368000	2.227611000
C	12.867141000	-2.909989000	-1.361616000	C	13.628352000	-2.526118000	-0.243459000
C	13.013945000	-1.696305000	0.722262000	C	11.706546000	-1.257500000	0.555127000
C	10.939422000	-1.664067000	-0.552219000	C	11.543365000	-2.505229000	-1.499942000
C	-1.795755000	4.005459000	-0.024760000	C	-1.186320000	5.084286000	-0.699593000
C	0.196586000	5.183777000	-0.766678000	C	1.024002000	4.199756000	-0.192327000
C	0.413659000	3.120983000	0.482642000	C	-0.969074000	3.021109000	0.549524000

H	-3.608897000	5.886800000	0.084238000	H	-5.473659000	2.570083000	0.154173000
H	-6.257981000	6.716849000	0.189466000	H	-8.621219000	5.388603000	0.287478000
H	-10.175446000	3.622727000	-0.132171000	H	-11.331046000	1.200578000	0.123671000
H	-4.976837000	-1.572277000	1.611440000	H	-6.059343000	-4.073794000	1.691774000
H	-8.696215000	-3.751537000	1.142173000	H	-15.406558000	-5.321372000	0.767088000
H	-13.697391000	-5.336752000	1.241530000	H	-14.877333000	-4.411123000	2.205236000
H	-16.907388000	-3.724844000	1.129710000	H	-18.832057000	-2.588442000	0.109165000
H	-18.505726000	-1.051191000	-1.828894000	H	-16.211820000	-0.685508000	-2.723652000
H	-12.569486000	-3.770146000	2.327220000	H	-11.174315000	-0.685705000	-1.285583000
H	-10.397464000	-2.638888000	2.458437000	H	2.811854000	2.320575000	-0.303270000
H	5.151885000	1.430100000	-0.307746000	H	5.059858000	5.654940000	-0.404930000
H	7.647320000	4.822299000	-0.461504000	H	9.518102000	3.378596000	0.015120000
H	11.109854000	1.209827000	-0.151777000	H	5.429144000	-2.725249000	-1.743959000
H	6.956009000	-4.982801000	-1.725527000	H	9.466205000	-4.168231000	-1.096336000
H	16.329405000	-4.473703000	-0.429875000	H	14.672122000	-4.813476000	-0.963005000
H	15.705189000	-3.719109000	-1.918863000	H	17.529058000	-2.640193000	-0.807816000
H	19.175406000	-1.140817000	0.230068000	H	18.502524000	0.369337000	2.099086000
H	16.148718000	0.336409000	2.907432000	H	13.313860000	-3.517881000	-2.138656000
H	11.254059000	-0.629448000	1.314652000	H	10.981006000	-2.807082000	-2.376136000
H	-1.804947000	5.830208000	-1.189190000	H	0.669452000	6.010473000	-1.287857000
H	1.031202000	2.375388000	0.973943000	H	-1.442857000	2.194689000	1.070171000

Table S16. S_0 optimized geometry of compound **6.SO$_2$** at B3LYP/6-31g (d,p) level of theory

Sum of imaginary frequencies= 0

Total Energy (Hartree) = -4405.894275

Atom	X	Y	Z	Atom	X	Y	Z
N	-3.187165000	3.941070000	0.122347000	C	-3.977794000	4.961506000	0.123262000
F	-6.400703000	1.275834000	2.475244000	F	-5.689292000	0.876018000	0.340325000
B	-6.745315000	0.693990000	1.260752000	N	-6.001246000	3.570682000	0.300688000
C	-5.404162000	4.798890000	0.220087000	C	-6.417370000	5.768855000	0.246805000
C	-7.638831000	5.094754000	0.335995000	C	-7.363180000	3.712864000	0.372642000
N	-8.066723000	1.327363000	0.718161000	C	-8.320226000	2.643183000	0.451798000
C	-9.720453000	2.815056000	0.256143000	C	-10.317114000	1.585274000	0.411833000
N	-6.998193000	-0.820209000	1.414409000	C	-6.057815000	-1.755427000	1.671340000
C	-6.647217000	-3.026723000	1.721368000	C	-8.008708000	-2.850729000	1.474838000
C	-9.288750000	0.643020000	0.692750000	C	-8.224066000	-1.464030000	1.289404000
C	-9.384016000	-0.731192000	0.954561000	C	-14.789530000	-4.397377000	1.720202000
C	-16.874577000	-2.941348000	0.404073000	C	-17.904269000	-2.343129000	-0.315350000
C	-17.644126000	-1.559450000	-1.444293000	C	-16.329268000	-1.395449000	-1.861605000
N	-14.480647000	-3.344975000	0.747116000	C	-15.533653000	-2.788600000	0.000875000
C	-15.295834000	-2.016373000	-1.155910000	S	-13.653944000	-1.947919000	-1.806437000
C	-12.369737000	-2.877246000	1.899001000	C	-13.218999000	-2.751011000	0.779190000
C	-12.741070000	-1.960400000	-0.289579000	C	-11.520238000	-1.293092000	-0.237802000
C	-10.690648000	-1.419994000	0.881213000	C	-11.139274000	-2.239565000	1.936779000
N	2.398240000	4.447961000	-0.395155000	C	3.180677000	3.422644000	-0.418480000
F	6.328093000	0.268811000	-2.635238000	F	5.641583000	-0.222998000	-0.512424000
B	6.744659000	-0.217425000	-1.401557000	N	5.441596000	2.477754000	-0.529238000
C	4.612585000	3.568918000	-0.487322000	C	5.421799000	4.715941000	-0.517598000
C	6.749961000	4.290617000	-0.566855000	C	6.751966000	2.880120000	-0.574389000
N	7.902022000	0.665195000	-0.836508000	C	7.894960000	2.011369000	-0.600186000
C	9.230793000	2.448187000	-0.367557000	C	10.051934000	1.349266000	-0.467154000
N	7.282391000	-1.657256000	-1.513919000	C	6.545064000	-2.757480000	-1.784109000
C	7.363851000	-3.894877000	-1.782083000	C	8.657437000	-3.461352000	-1.489001000
C	9.229326000	0.223586000	-0.752329000	C	8.601150000	-2.056854000	-1.328455000
C	9.589886000	-1.112380000	-0.972167000	C	15.621725000	-3.692027000	-1.438758000
C	17.329085000	-1.849952000	-0.064309000	C	18.192666000	-1.058399000	0.686233000
C	17.737803000	-0.327657000	1.788712000	C	16.398550000	-0.414172000	2.147673000
N	15.074136000	-2.708648000	-0.499226000	C	15.967132000	-1.952906000	0.279748000
C	15.535122000	-1.228679000	1.411114000	S	13.882470000	-1.469042000	1.989393000
C	12.965521000	-2.668875000	-1.746500000	C	13.725116000	-2.367343000	-0.596076000
C	13.058885000	-1.668272000	0.435056000	C	11.738029000	-1.244172000	0.317782000
C	10.998275000	-1.541492000	-0.831449000	C	11.639392000	-2.277143000	-1.848618000
C	-1.804578000	4.108471000	-0.028504000	C	-1.200566000	5.165141000	-0.741342000
C	0.181375000	5.251959000	-0.836257000	C	1.014979000	4.276957000	-0.255537000
C	0.410726000	3.219257000	0.455469000	C	-0.971337000	3.133286000	0.551543000

H	-3.622901000	5.997207000	0.069884000	H	-5.506692000	2.682834000	0.269513000
H	-6.261514000	6.837708000	0.207154000	H	-8.621426000	5.539734000	0.392037000
H	-10.204158000	3.748758000	0.010731000	H	-11.370339000	1.360562000	0.338658000
H	-5.021008000	-1.476801000	1.797167000	H	-6.128573000	-3.956867000	1.903798000
H	-8.764937000	-3.618812000	1.408875000	H	-15.570857000	-5.038058000	1.312604000
H	-13.903114000	-5.012417000	1.872745000	H	-15.120110000	-3.996042000	2.685066000
H	-17.114771000	-3.500501000	1.298967000	H	-18.925598000	-2.475048000	0.027669000
H	-18.454459000	-1.086839000	-1.988069000	H	-16.084678000	-0.798482000	-2.733598000
H	-12.688642000	-3.441887000	2.765184000	H	-11.209803000	-0.705423000	-1.094420000
H	-10.528207000	-2.338785000	2.827147000	H	2.802752000	2.391764000	-0.402587000
H	5.158282000	1.501958000	-0.476021000	H	5.054014000	5.730935000	-0.507595000
H	7.628479000	4.917588000	-0.614319000	H	9.521378000	3.461860000	-0.135026000
H	11.125184000	1.327906000	-0.353567000	H	5.480561000	-2.681379000	-1.955685000
H	7.037243000	-4.908896000	-1.962503000	H	9.541262000	-4.071874000	-1.377890000
H	16.492584000	-4.166474000	-0.987504000	H	14.877036000	-4.467282000	-1.616530000
H	15.911667000	-3.244501000	-2.396328000	H	17.710623000	-2.361468000	-0.938309000
H	19.234603000	-0.995899000	0.388587000	H	18.418040000	0.296902000	2.356962000
H	16.005961000	0.133865000	2.997387000	H	13.423473000	-3.175306000	-2.585972000
H	11.284418000	-0.713626000	1.147448000	H	11.097670000	-2.504385000	-2.760179000
H	-1.817115000	5.906211000	-1.240268000	H	0.646365000	6.064324000	-1.386174000
H	1.027627000	2.479039000	0.955250000	H	-1.436818000	2.321935000	1.102439000
O	-13.436358000	-0.672971000	-2.518505000	O	-13.372166000	-3.199244000	-2.543687000
O	13.810097000	-2.745634000	2.733627000	O	13.394074000	-0.253500000	2.670392000

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