Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Synthesis of Unsymmetrical 2,3,7,8-Tetrabromo *Meso*-5,10,11,16-Tetraaryl- Triphyrin(2.1.1) and Its Use in the Synthesis of Sterically Crowded 2,3,5,7,8,10,11,16-Octaarylated Triphyrin(2.1.1)s

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General Experimental Section:

Materials and Methods: Reagent-grade chemicals were employed during synthesis. For column chromatography purification purpose, silica (60−120 and 100−200 mesh) and basic alumina was used. Bruker 400 and 500 MHz instruments assisted us in recording 1D, 2D and ^{13}C using $CDCl_3$ as solvent. 100.06 and 125.77 MHz is the frequency for the ^{13}C nucleus for 400 and 500 MHz respectively. For ^{1}H and $^{13}C\{^{1}H\}$ NMR the internal standard used was Tetramethylsilane [$Si(CH_3)_4$]. Structural assignments were made with additional information from COSY and NOESY experiments for compound **12**. Carry series UV−vis−NIR and UV 3600 Shimadzu spectrophotometer helped us to record the absorption spectra of the compounds. For UV−Vis stock solution (10^{-5} M) was prepared by using a HPLC grade chloroform solvent. Cyclic voltammetry (CV) studies were carried out with BASi C3 Cell Stand electrochemical system (Manufacturer: Bioanalytical Systems. Inc.) utilizing the three electrode configuration consisting of a glassy carbon (working electrode), platinum wire (auxiliary electrode) and saturated calomel as reference electrode (the electrode is composed of Hg/Hg_2C_{l2}/Saturated KCl solution). The experiments were done in dry dichloromethane using 0.1 M tetrabutylammonium perchlorate as supporting electrolyte. The initial and final potential was at 0 V, first switching potential at -2.0 V and second switching potential at 2.0 V. Glassy carbon-disk working electrodes (3 mm diameter, part # CHI 104) were purchased from CH Instruments, HRMS was recorded on a Bruker maXis Impact and LC-MS Q-Tof micro mass spectrometer using positive mode ESI methods for acetonitrile/methanol solutions.

X-ray Crystal Structure Analysis: Single crystal X-ray structure analysis was performed on on a Rigaku Saturn 724 diffractometer that was equipped with a low-temperature attachment. Data were collected at 100 K using graphite-monochromated Mo Kα radiation (λα =0.71073 Å) by the ω-scan technique. The data were reduced by using Crystal Clear-SM Expert 2.1

b24 software. The structures were solved by direct methods and refined by least-squares against F2 utilizing the software packages SHELXL-97,[1] SIR-92,[2] and WINGX. All nonhydrogen atoms were refined anisotropically. The X-ray data for the compound **8** were collected on a Bruker Kappa CCD diffractometer equipped with a graphite monochromated Mo Kα radiation source at 200 K using the θ–2θ scan mode. An empirical absorption correction by multi scans was applied and all of the non-hydrogen atoms were refined with anisotropic displacement factors. The hydrogen atoms were placed in ideal positions and fixed with relative isotropic displacement parameters. The single crystals of compound **8** were obtained by slow diffusion of n-hexane into chloroform solution over a period of 5-6 days. CCDC no. 2307843 contains the supplementary crystallographic data for this paper.

Computational details: For all the calculations Gaussian 09 program package was used.[3] The density functional theory (DFT)[4] method, hybrid functional B3LYP in conjunction with basis set 6-31G(d,p)[5] helped to optimize the structure of compounds **9-14** in the ground (S_0) states. To obtain the oscillator strengths, identical basis and functional hybrid set were used whereas the vertical excitation energies were obtained with the help of TD-DFT techniques for $S_0 \rightarrow S_n$ transitions.[6] Under the Polarizable Continuum Model (PCM) in the toluene media all the computations were done using the Self-Consistent Reaction Field (SCRF). The electronic absorption spectra as well as the oscillator strengths were thoroughly examined using TD-DFT with PCM model[7] on the basis of the optimized structures in the S_0 state.

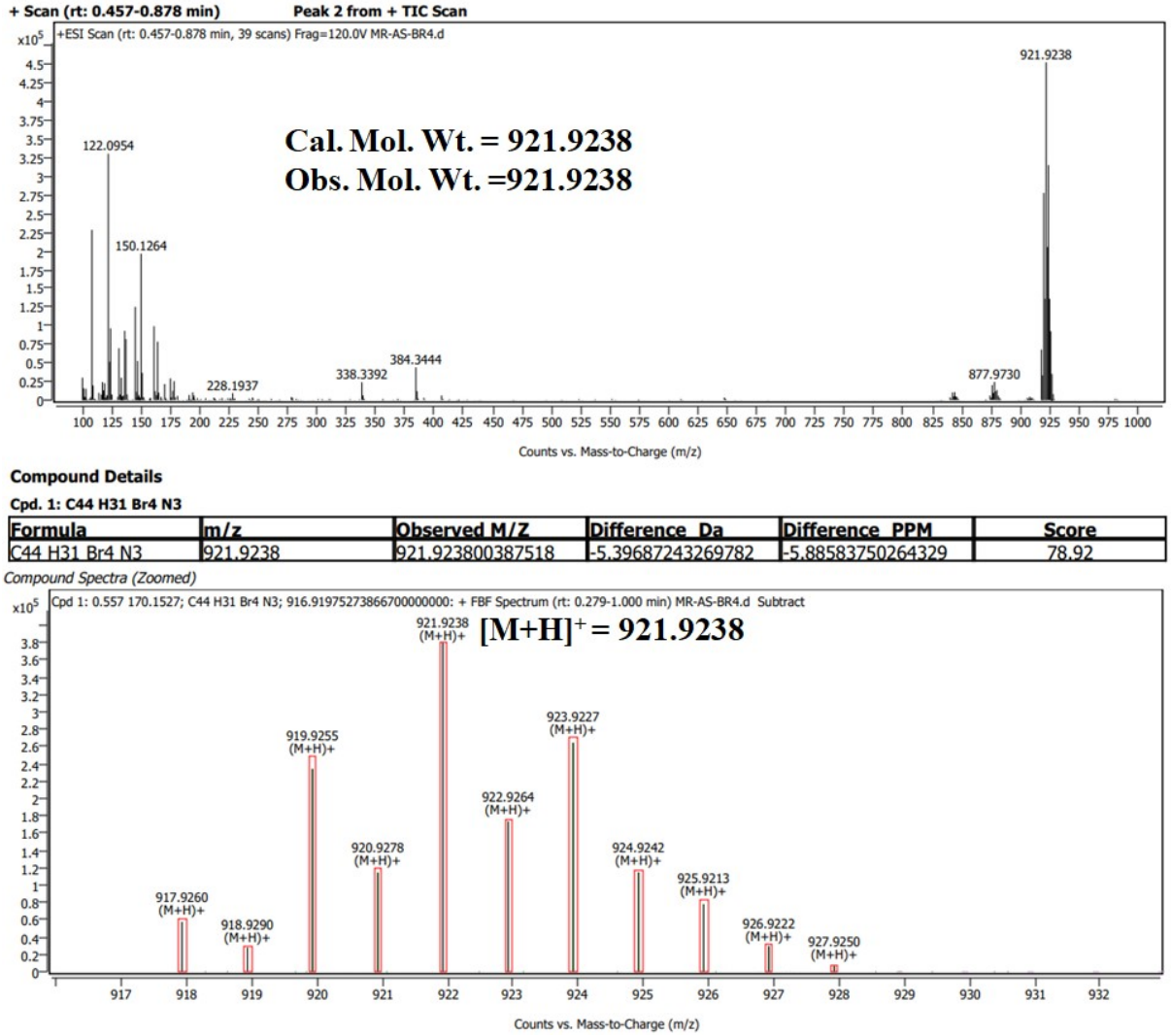

Figure S1. HR mass spectrum of the compound **8**.

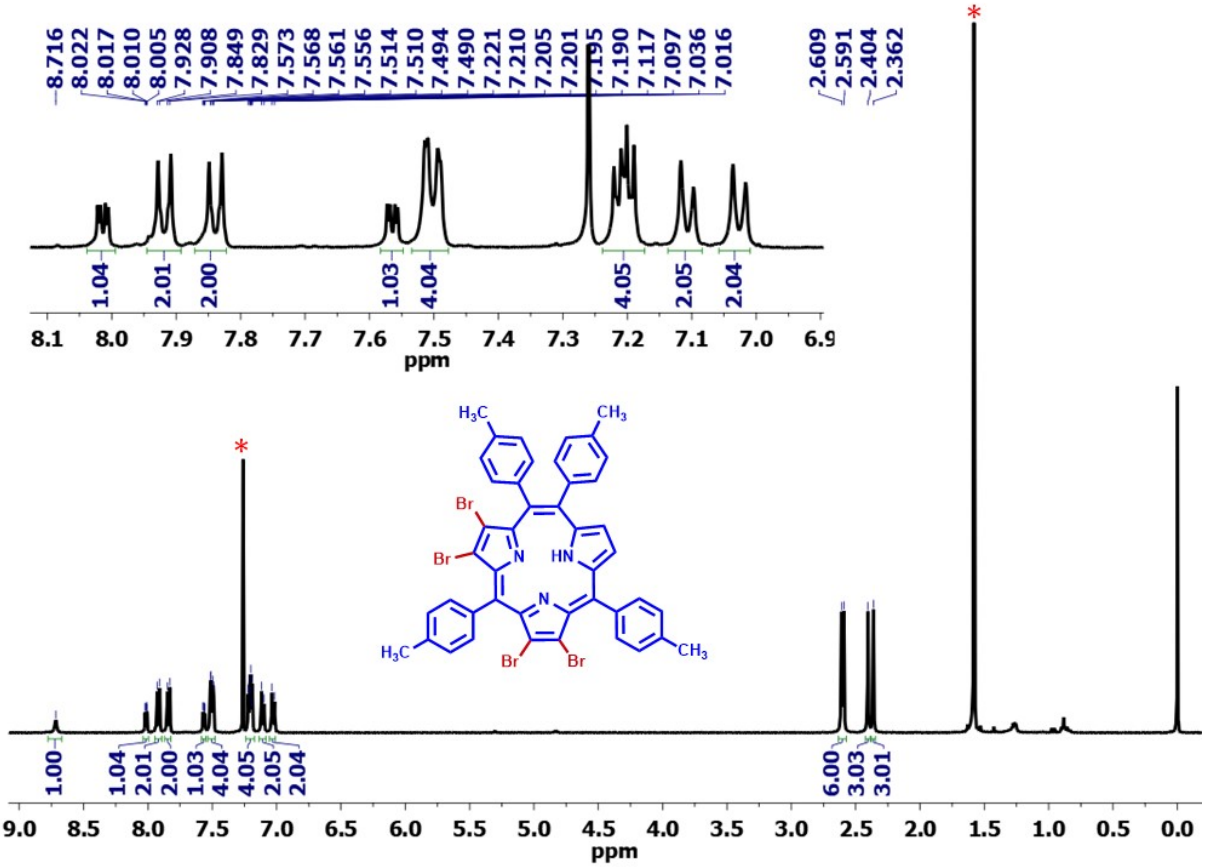

Figure S2. [1] H NMR spectrum of the compound **8** recorded in $CDCl_3$ on 400 MHz FT-NMR spectrometer. Note: Peaks marked with asterisk (*) are due to residual solvents.

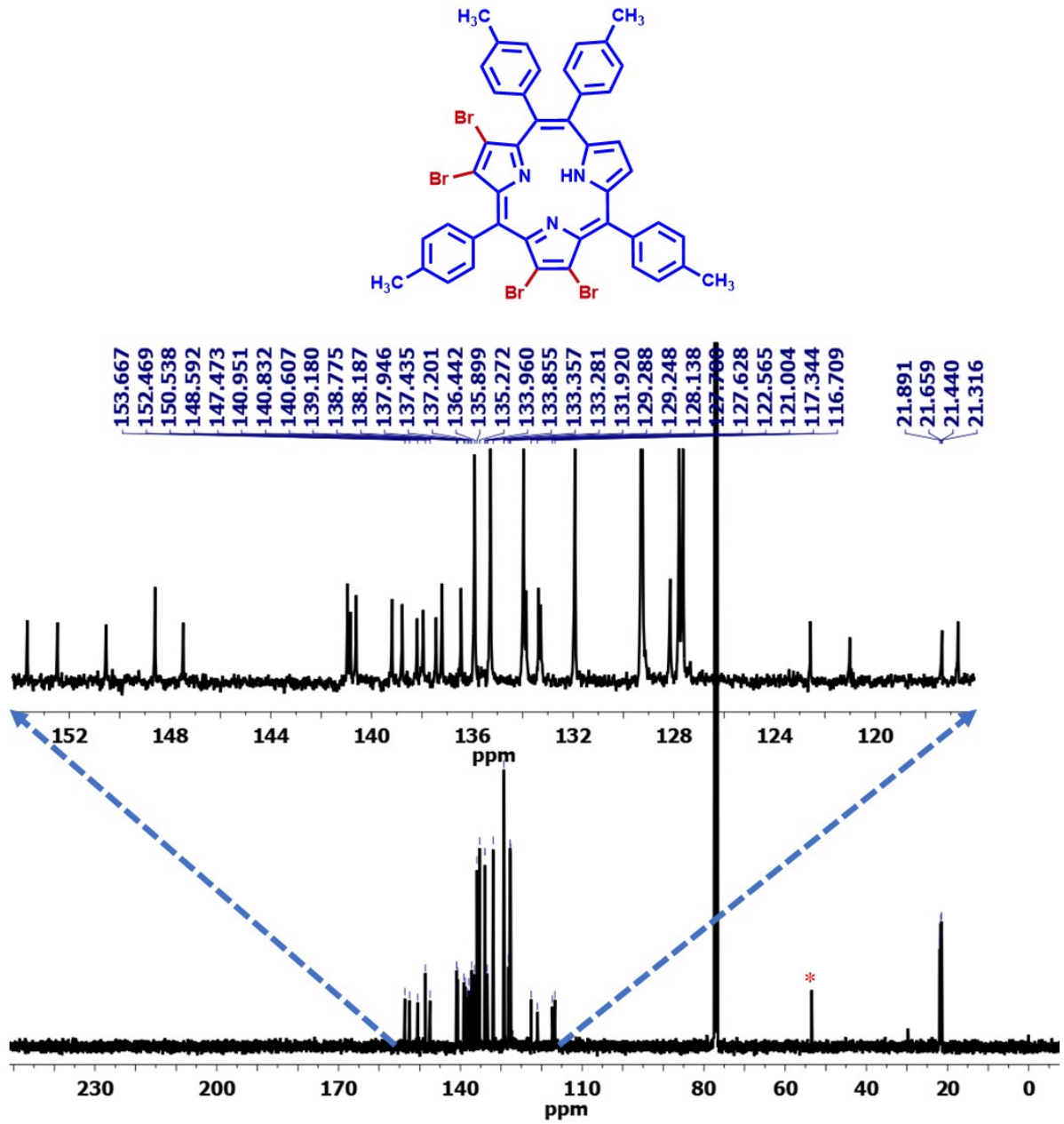

Figure S3. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **8** recorded in $CDCl_3$ on 101 MHz FT-NMR spectrometer. Note: Peaks marked with asterisk (*) are due to residual solvents.

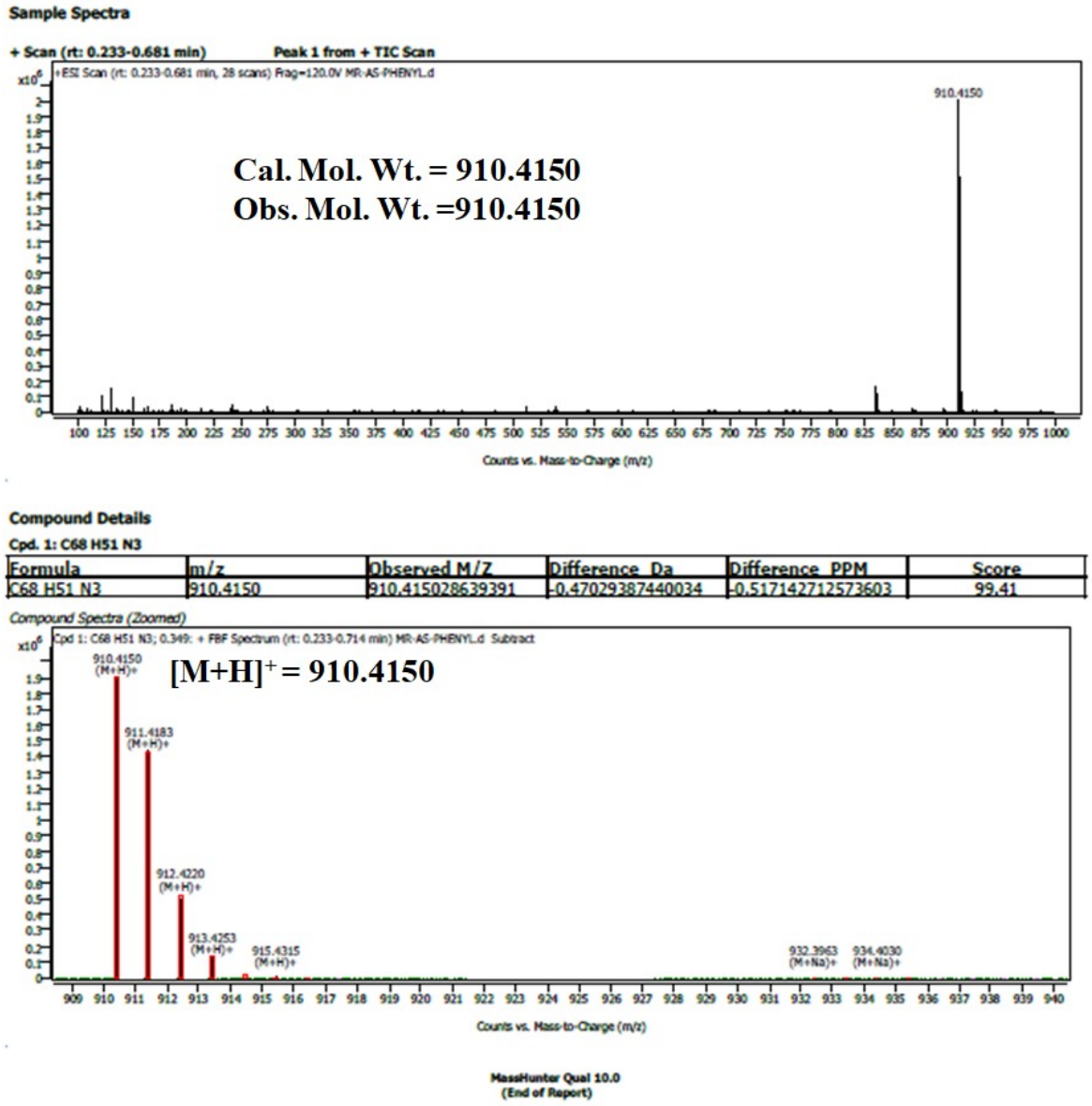

Figure S4. HR mass spectrum of the compound **9**.

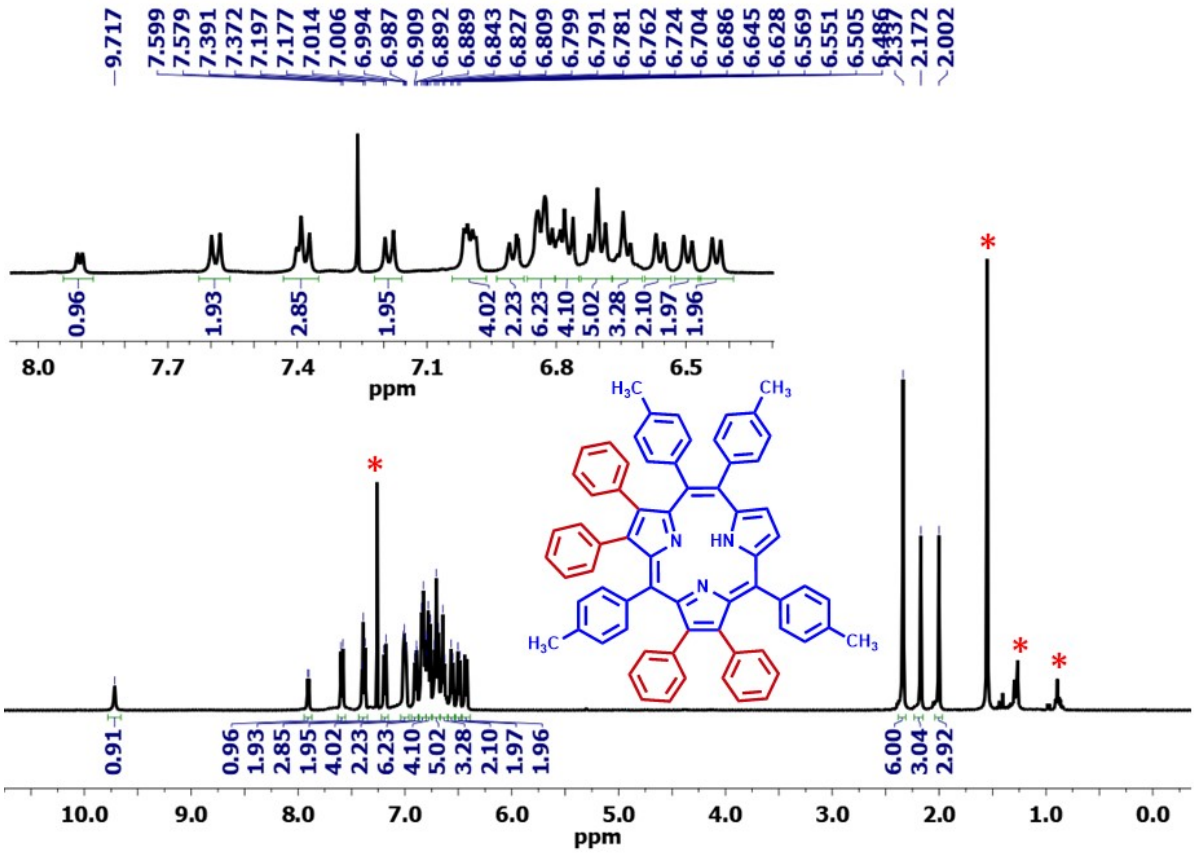

Figure S5. [1] H NMR spectrum of the compound **9** recorded in $CDCl_3$ on 400 MHz FT-NMR spectrometer. Note: Peaks marked with asterisk (*) are due to residual solvents.

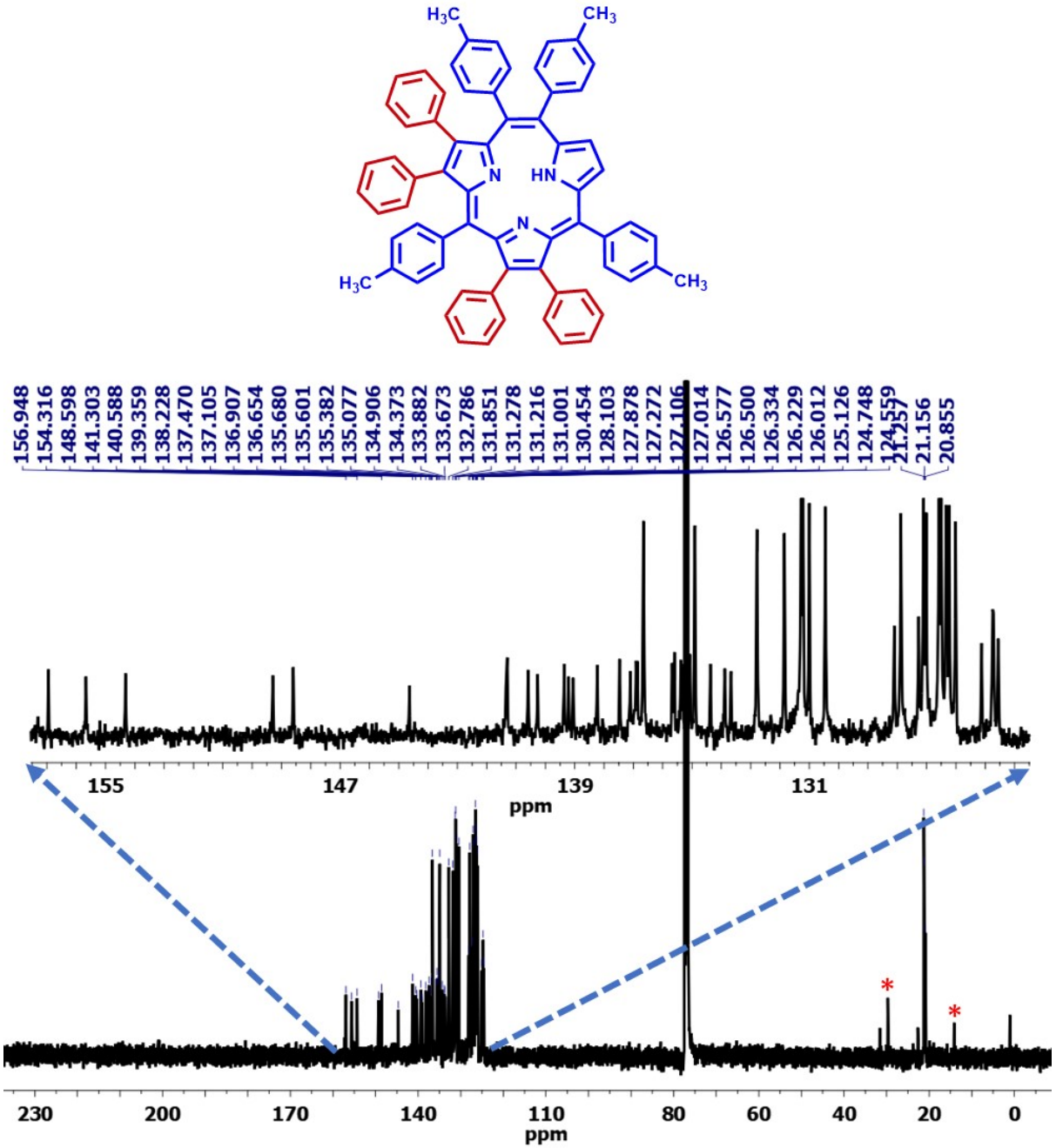

Figure S6. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **9** recorded in $CDCl_3$ on 101 MHz FT-NMR spectrometer. Note: Peaks marked with asterisk (*) are due to residual solvents.

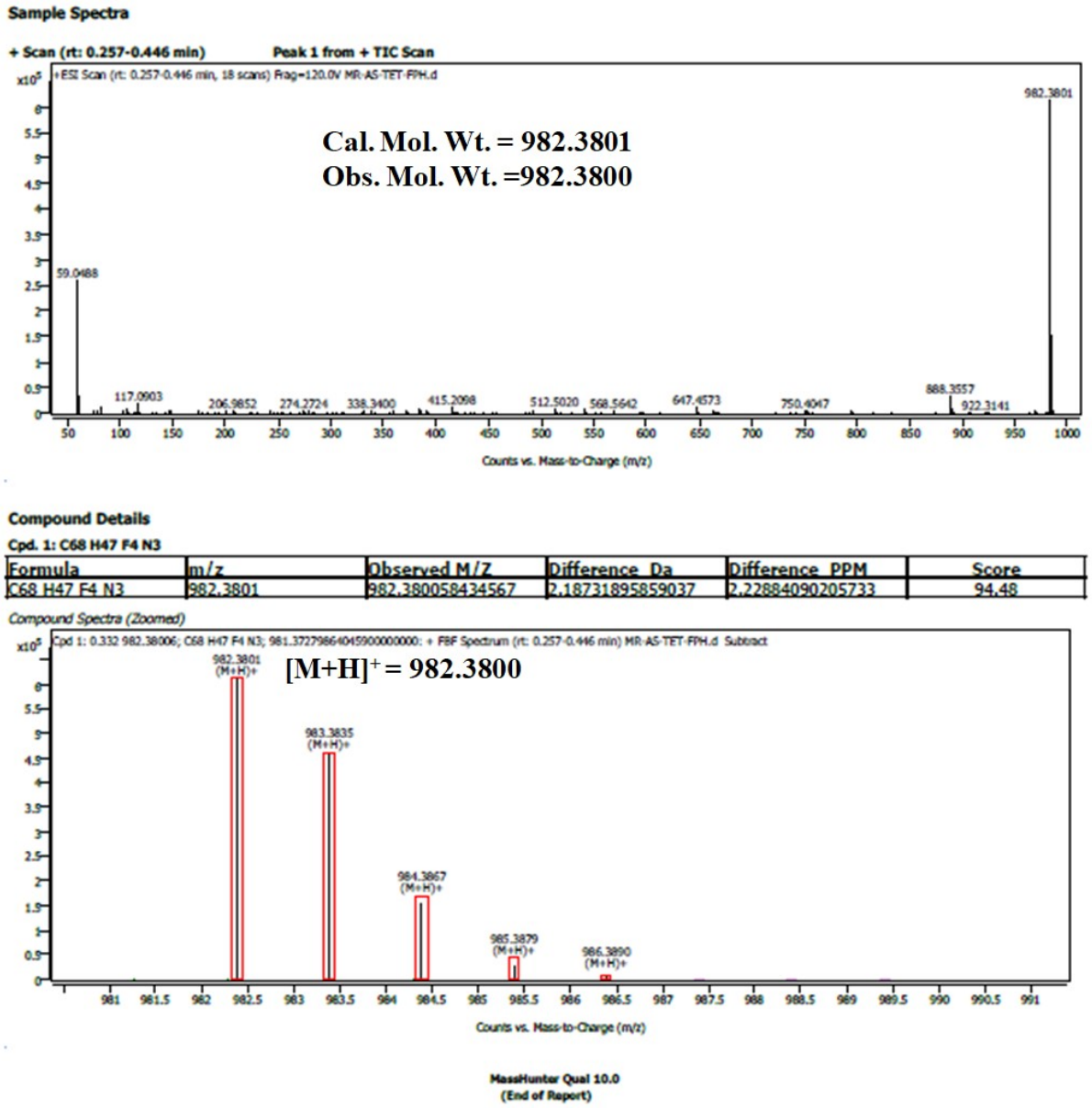

Figure S7. HR mass spectrum of the compound **10**.

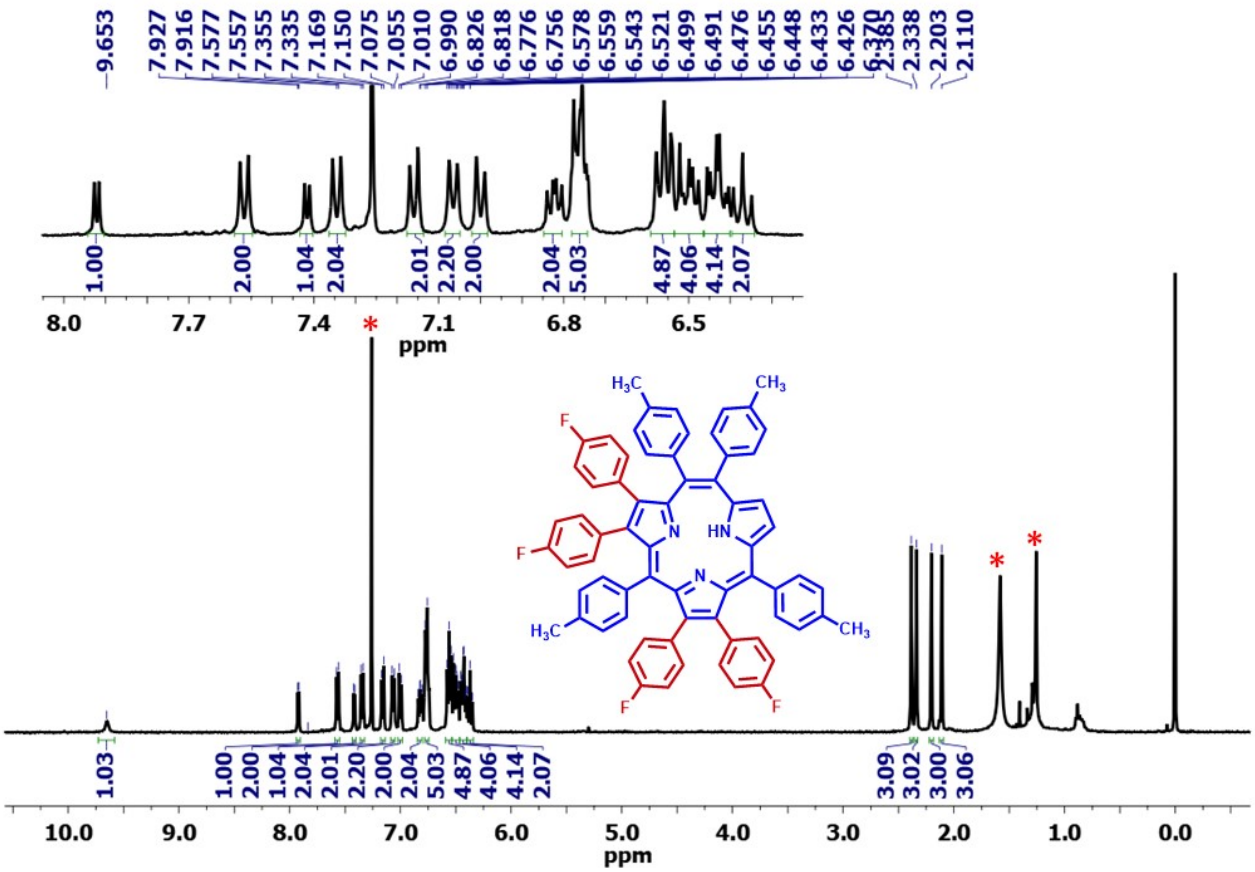

Figure S8. [1] H NMR spectrum of the compound **10** recorded in $CDCl_3$ on 400 MHz FT-NMR spectrometer. Note: Peaks marked with asterisk (*) are due to residual solvents.

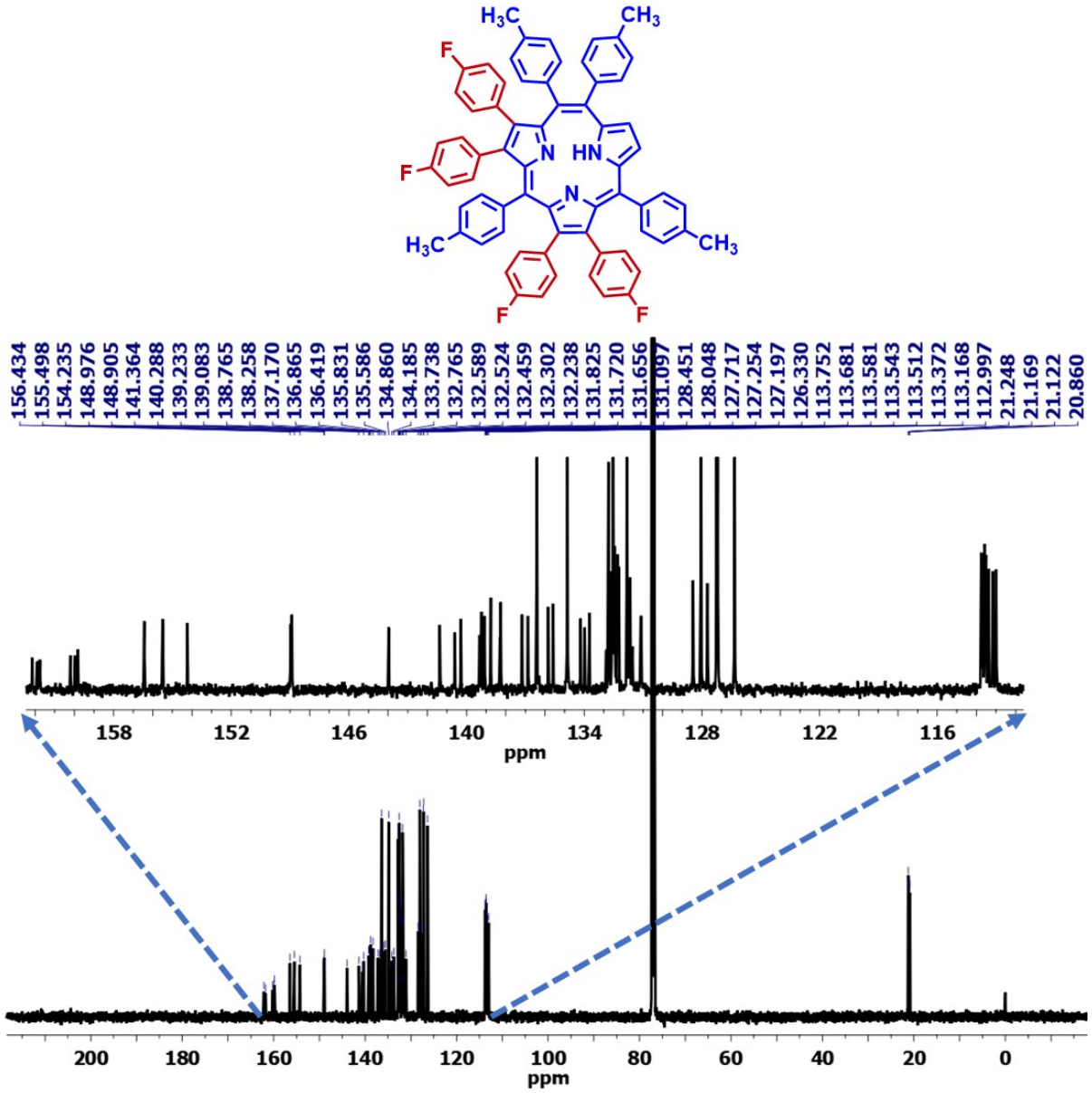

Figure S9. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **10** recorded in $CDCl_3$ on 101 MHz FT-NMR spectrometer.

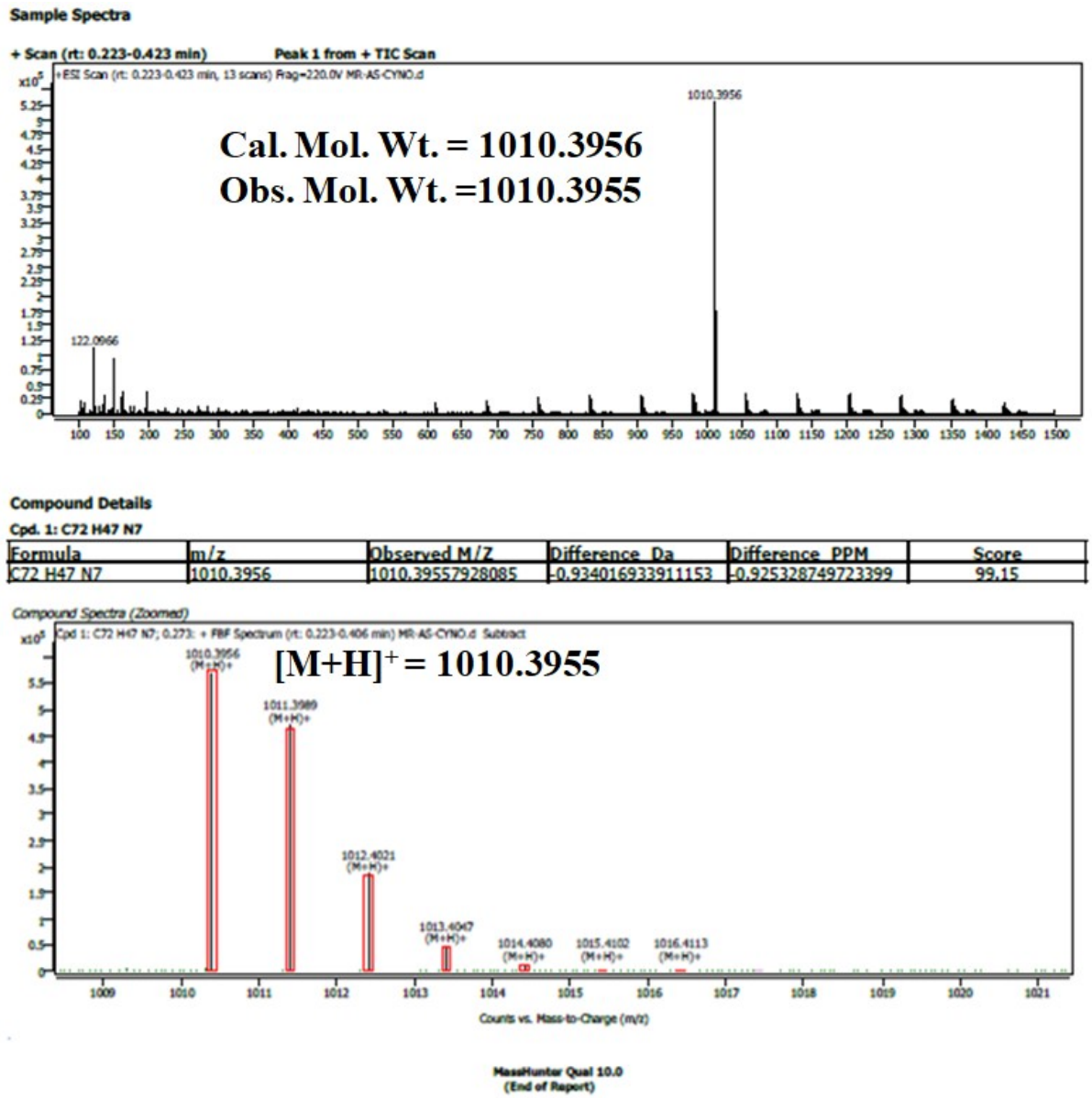

Figure S10. HR mass spectrum of the compound **11**.

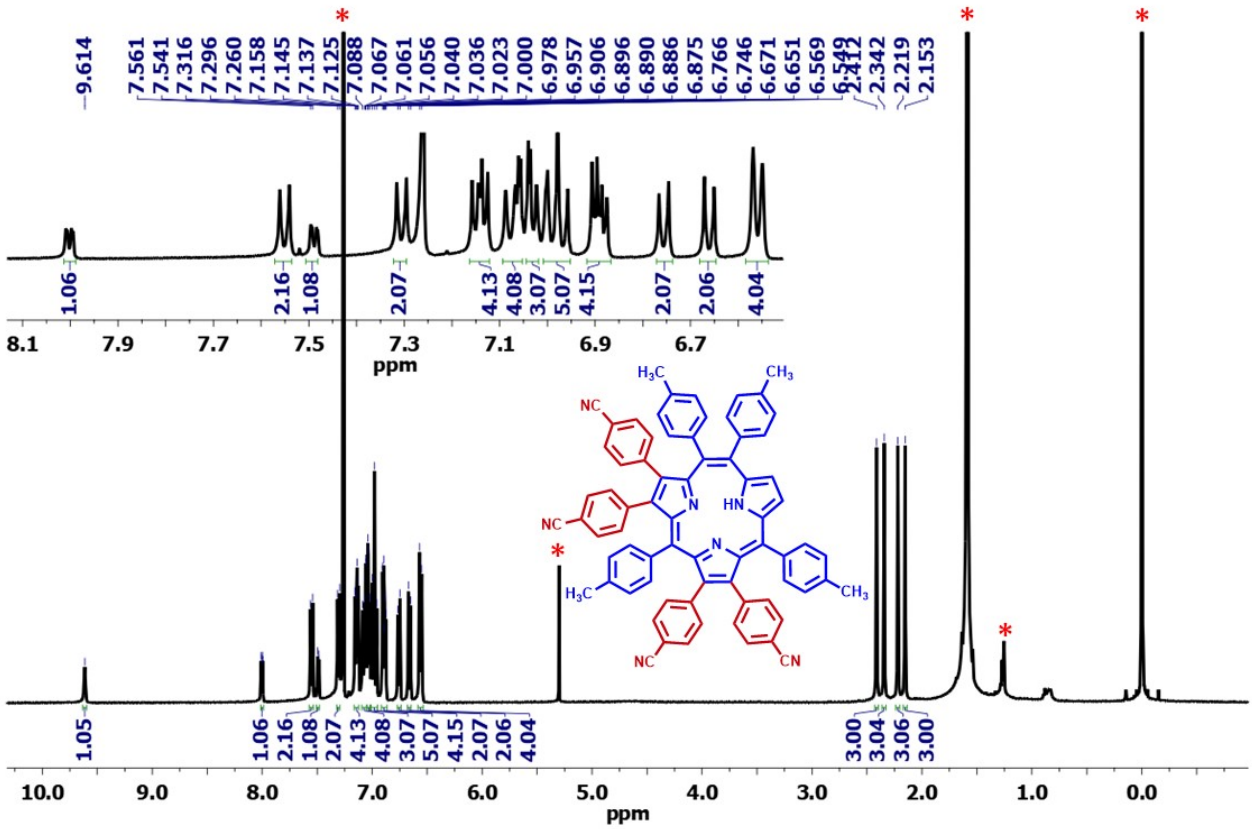

Figure S11. [1] H NMR spectrum of the compound **11** recorded in $CDCl_3$ on 400 MHz FT-NMR spectrometer. Note: Peaks marked with asterisk (*) are due to residual solvents.

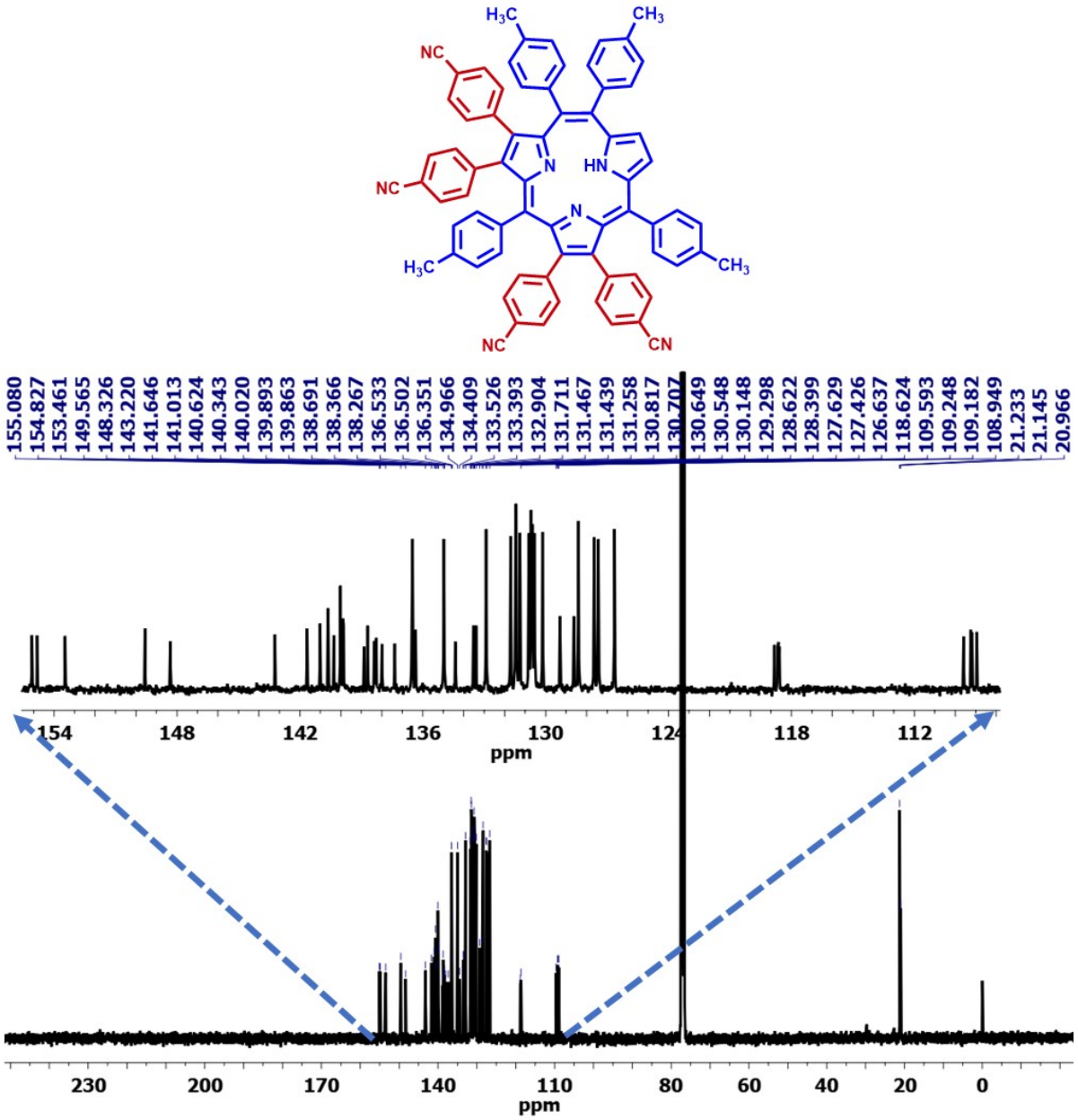

Figure S12. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **11** recorded in $CDCl_3$ on 101 MHz FT-NMR spectrometer.

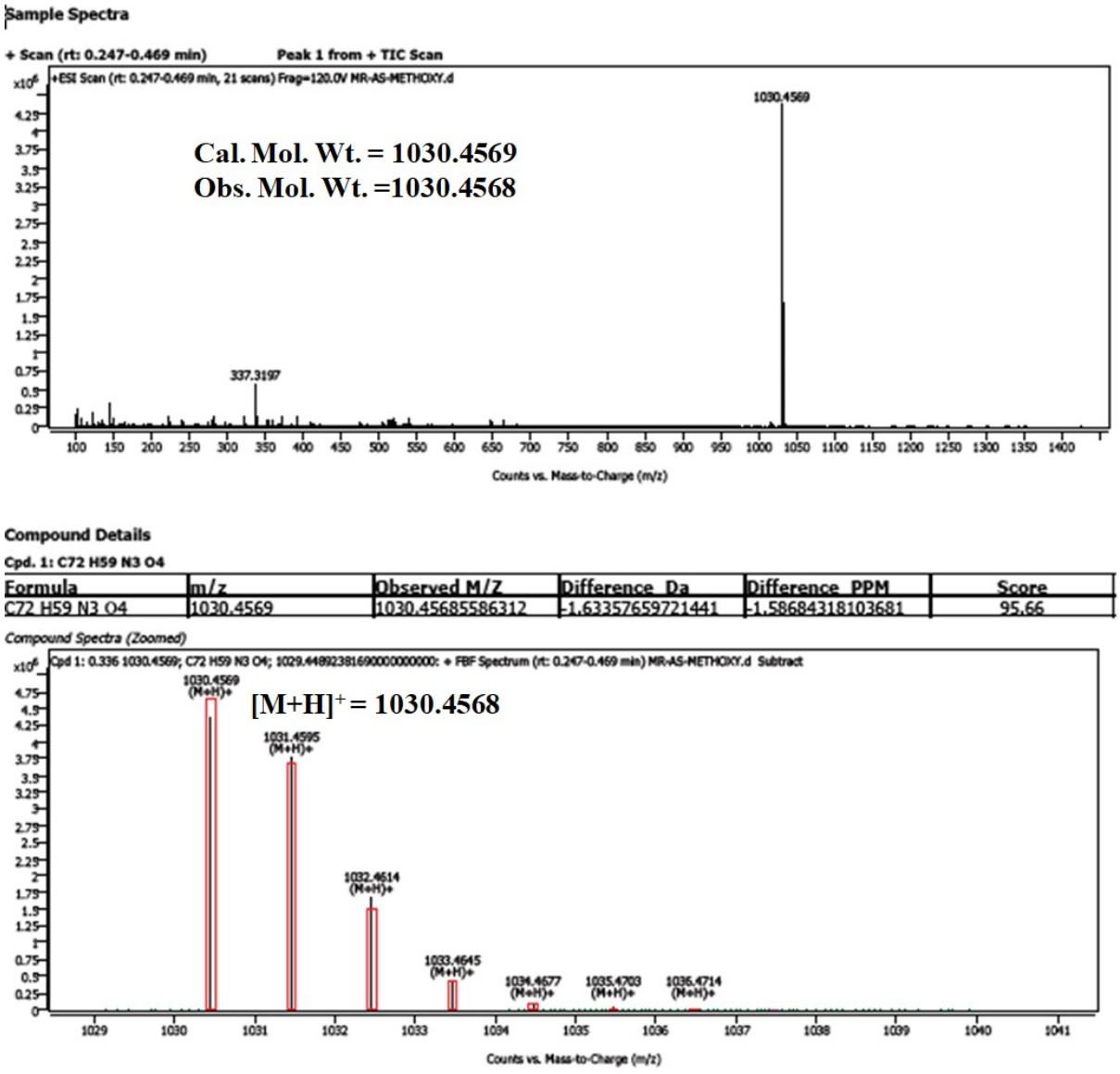

Figure S13. HR mass spectrum of the compound **12**.

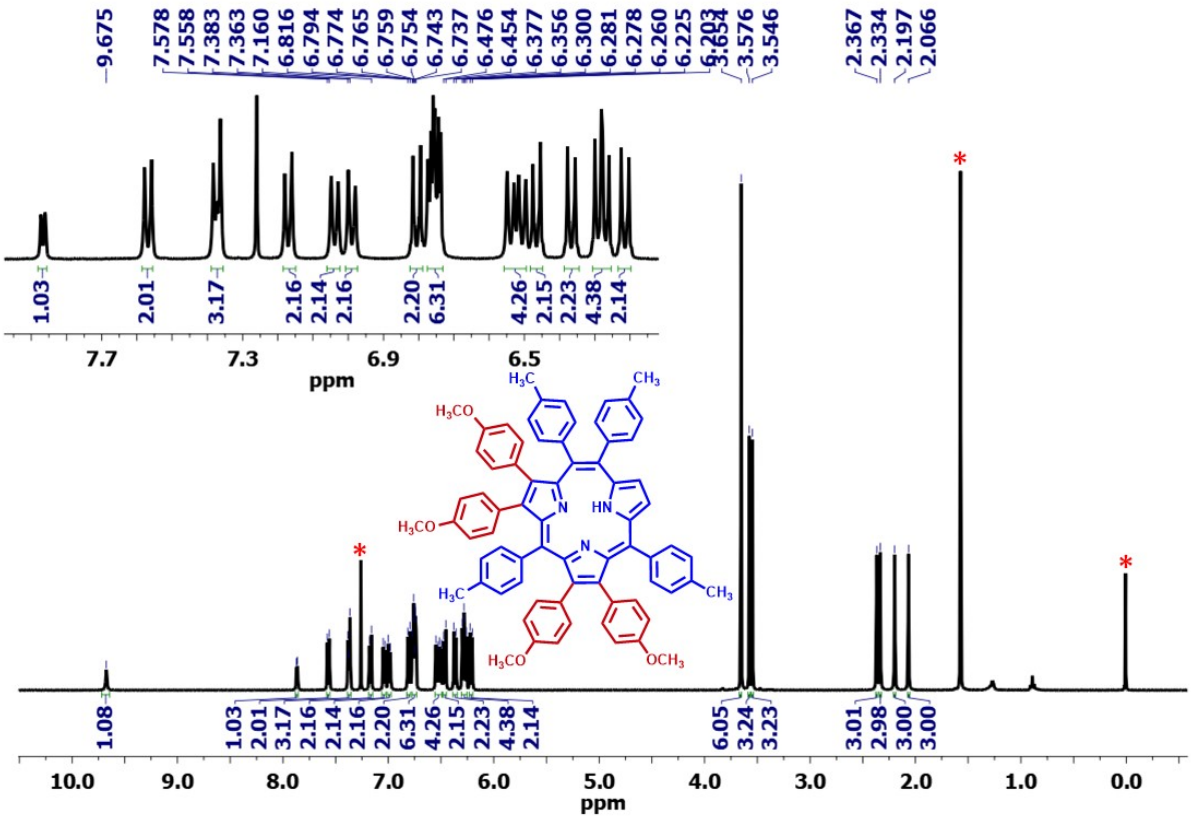

Figure S14. [1] H NMR spectrum of the compound **12** recorded in $CDCl_3$ on 400 MHz FT-NMR spectrometer. Note: Peaks marked with asterisk (*) are due to residual solvents.

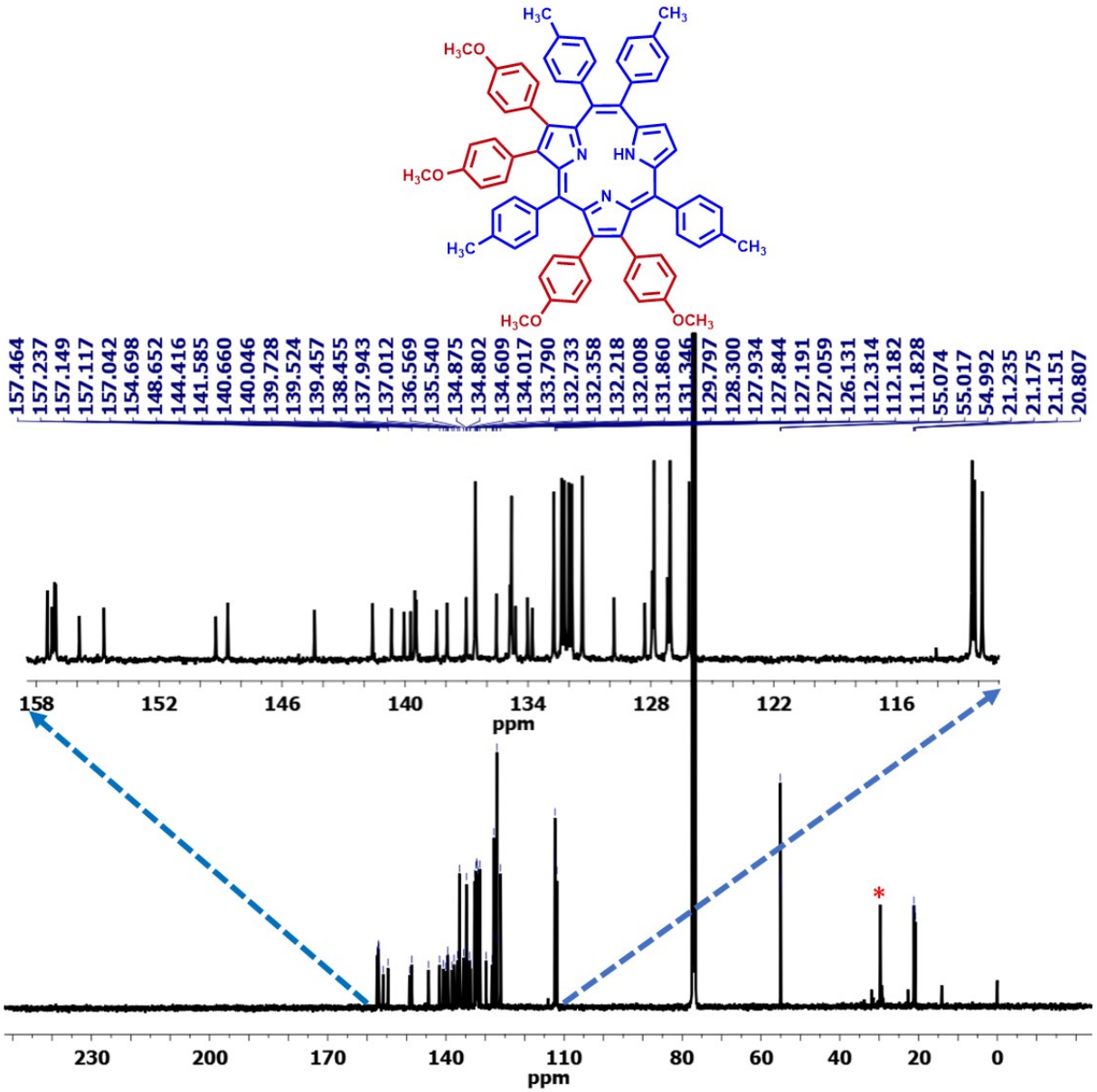

Figure S15. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **12** recorded in $CDCl_3$ on 101 MHz FT-NMR spectrometer. Note: Peaks marked with asterisk (*) are due to residual solvents.

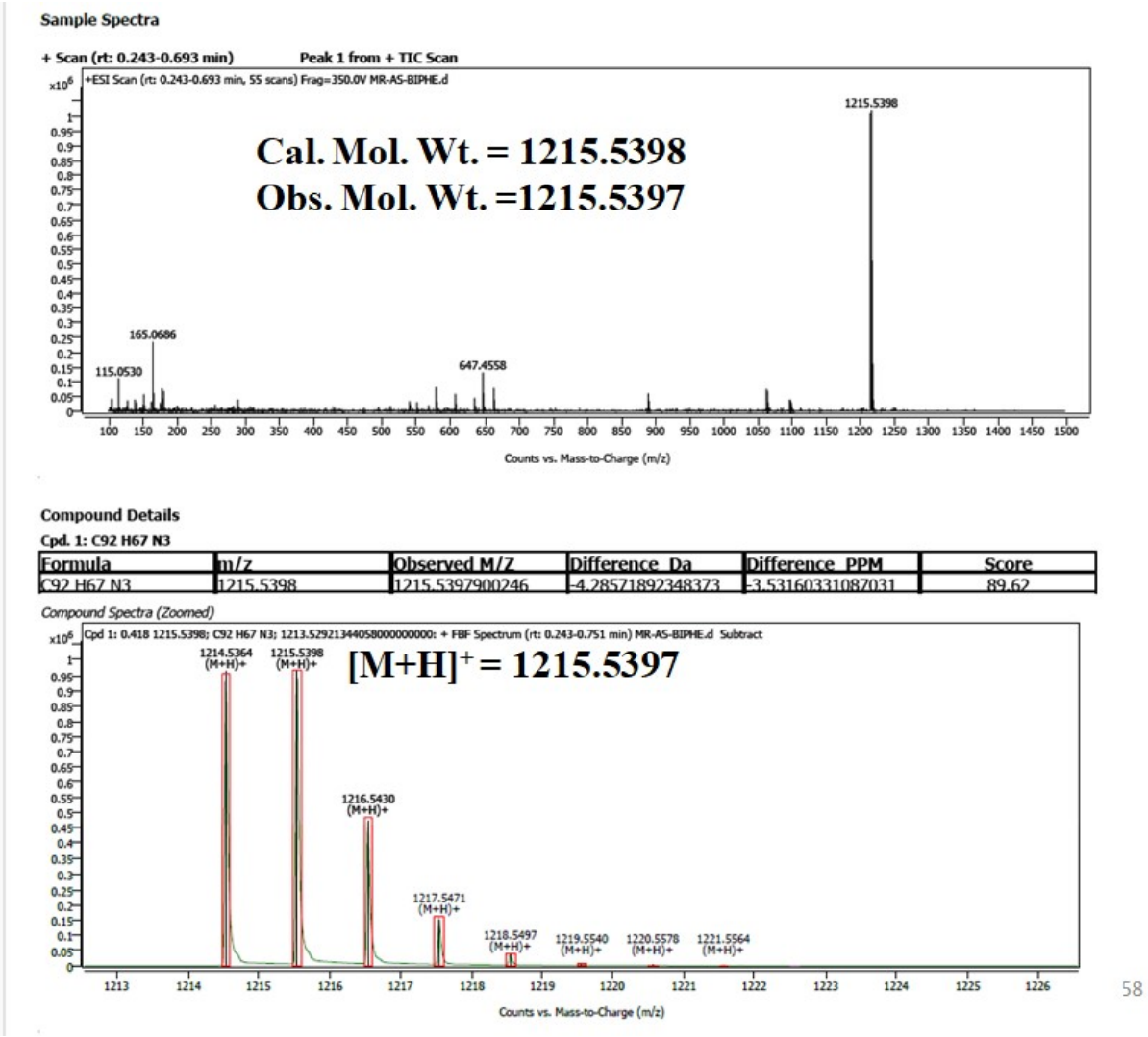

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Figure S16. HR mass spectrum of the compound **13**.

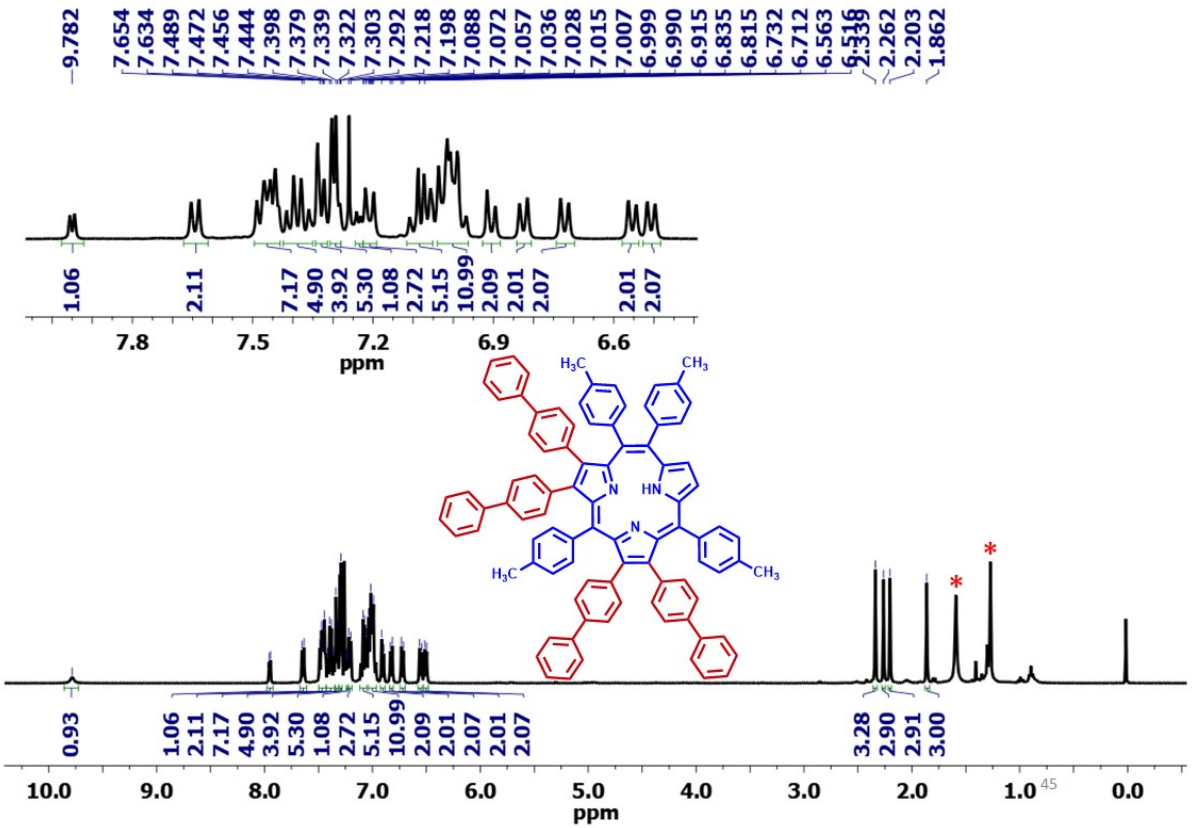

Figure S17. ^{1}H NMR spectrum of the compound **13** recorded in $CDCl_3$ on 400 MHz FT-NMR spectrometer. Note: Peaks marked with asterisk (*) are due to residual solvents.

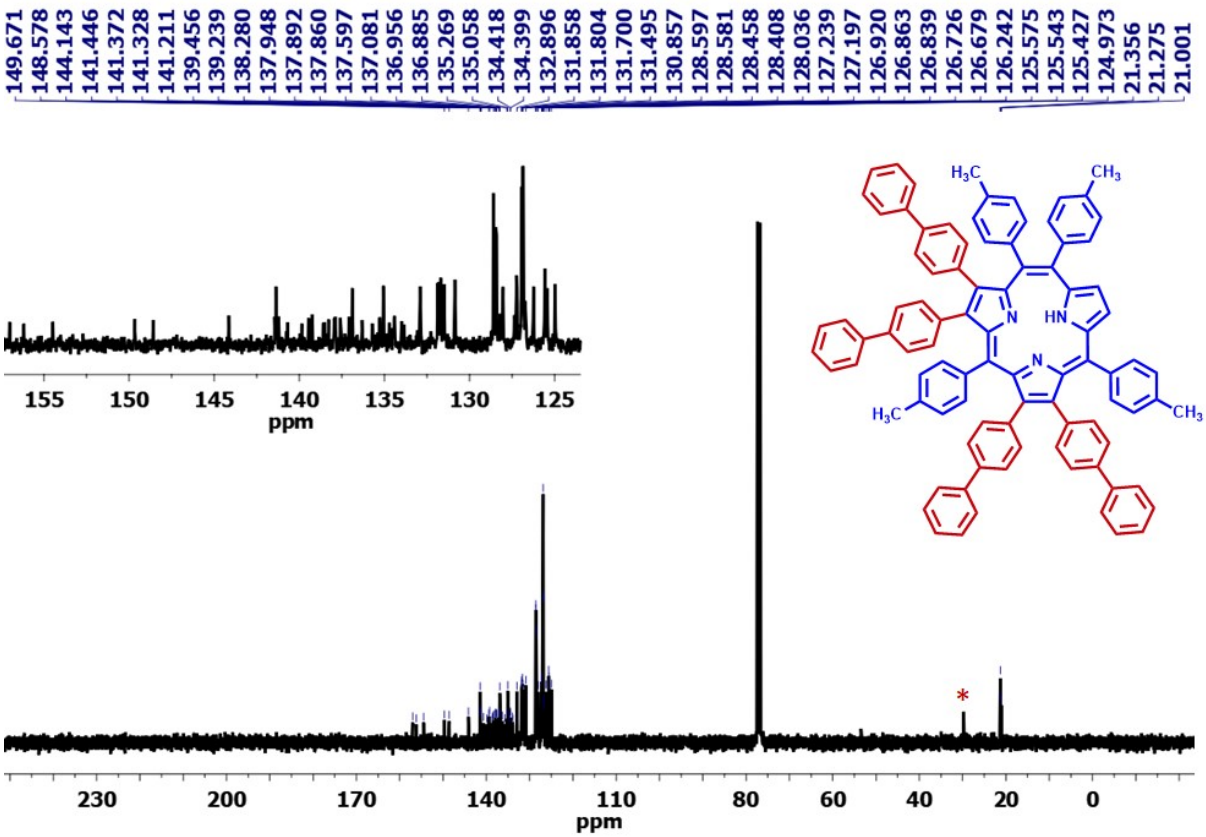

Figure S18. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **13** recorded in $CDCl_3$ on 101 MHz FT-NMR spectrometer. Note: Peaks marked with asterisk (*) are due to residual solvents.

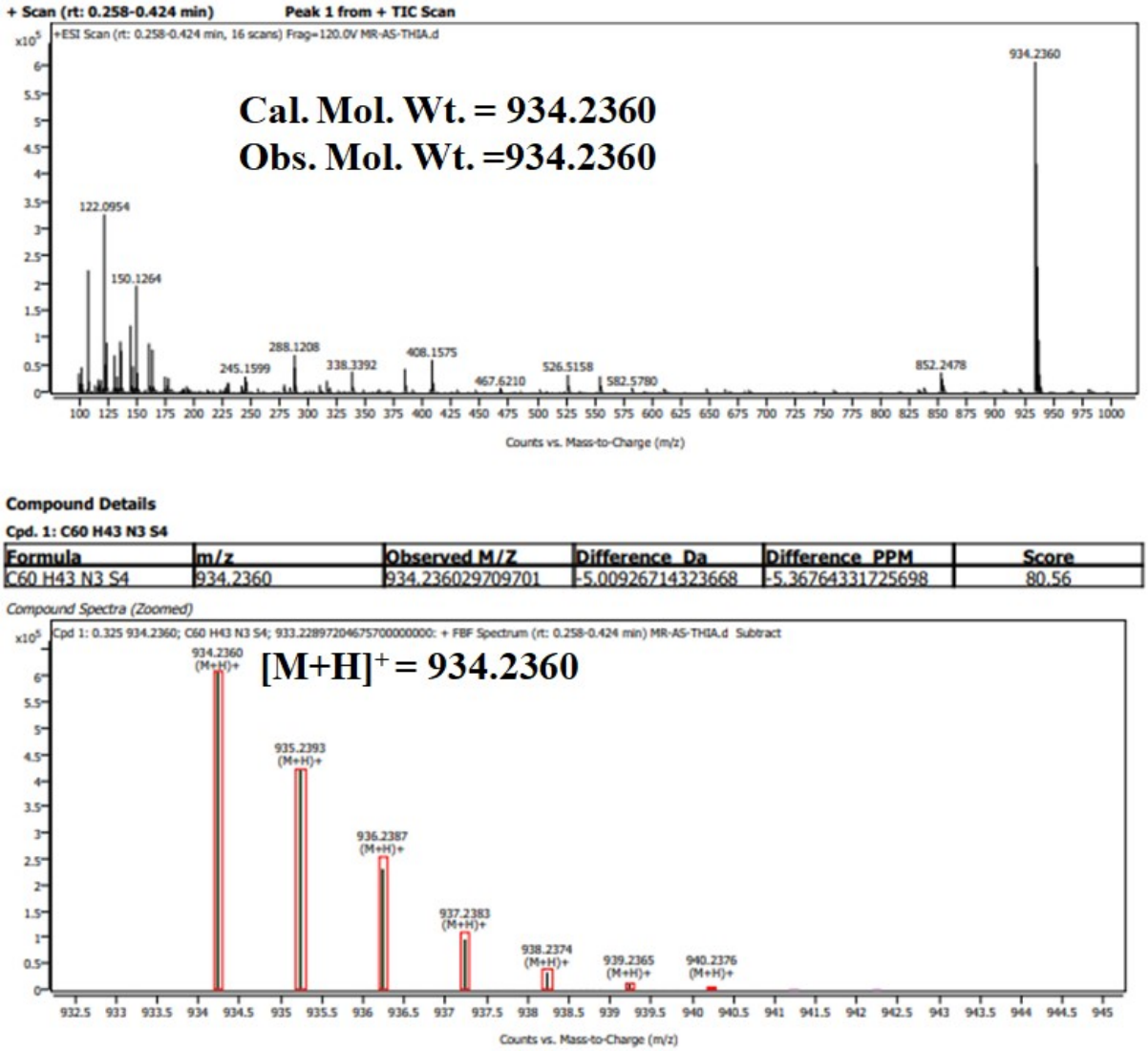

Figure S19. HR mass spectrum of the compound **14**.

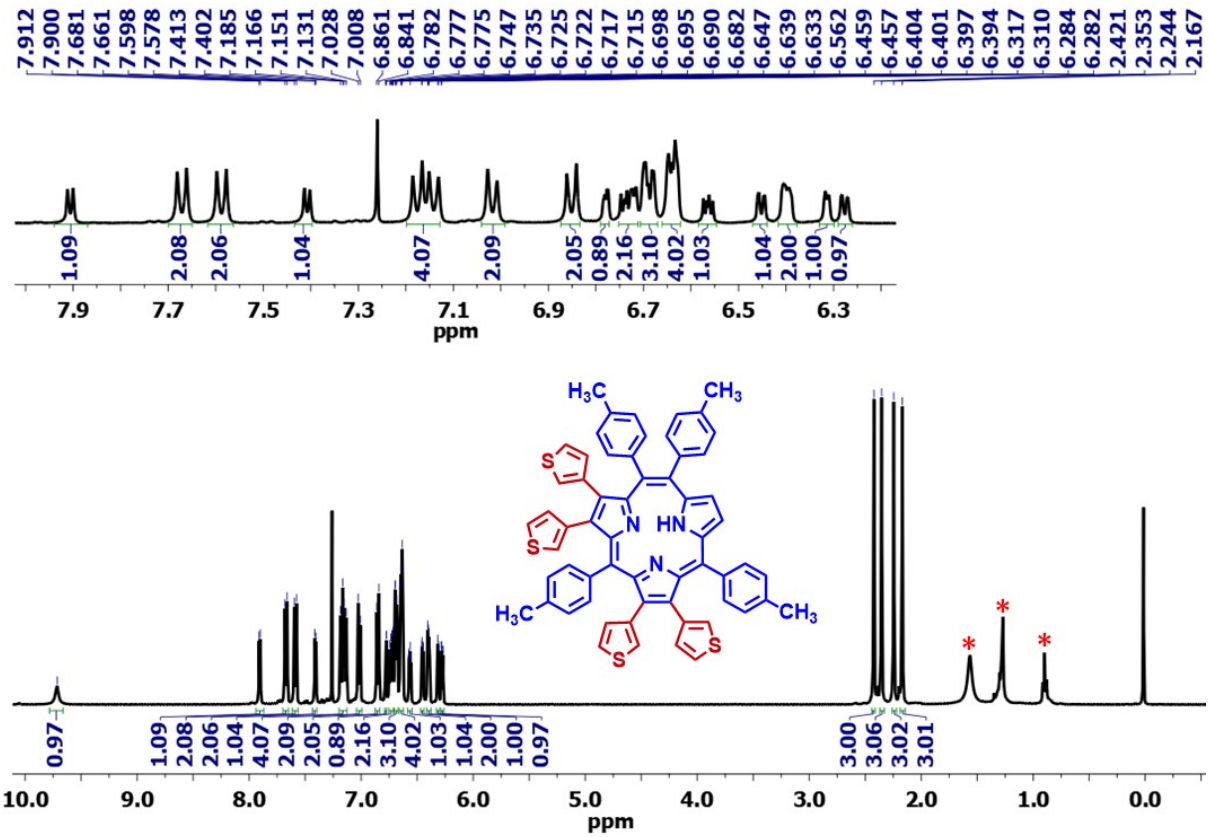

Figure S20. [1] H NMR spectrum of the compound **14** recorded in $CDCl_3$ on 400 MHz FT-NMR spectrometer. Note: Peaks marked with asterisk (*) are due to residual solvents.

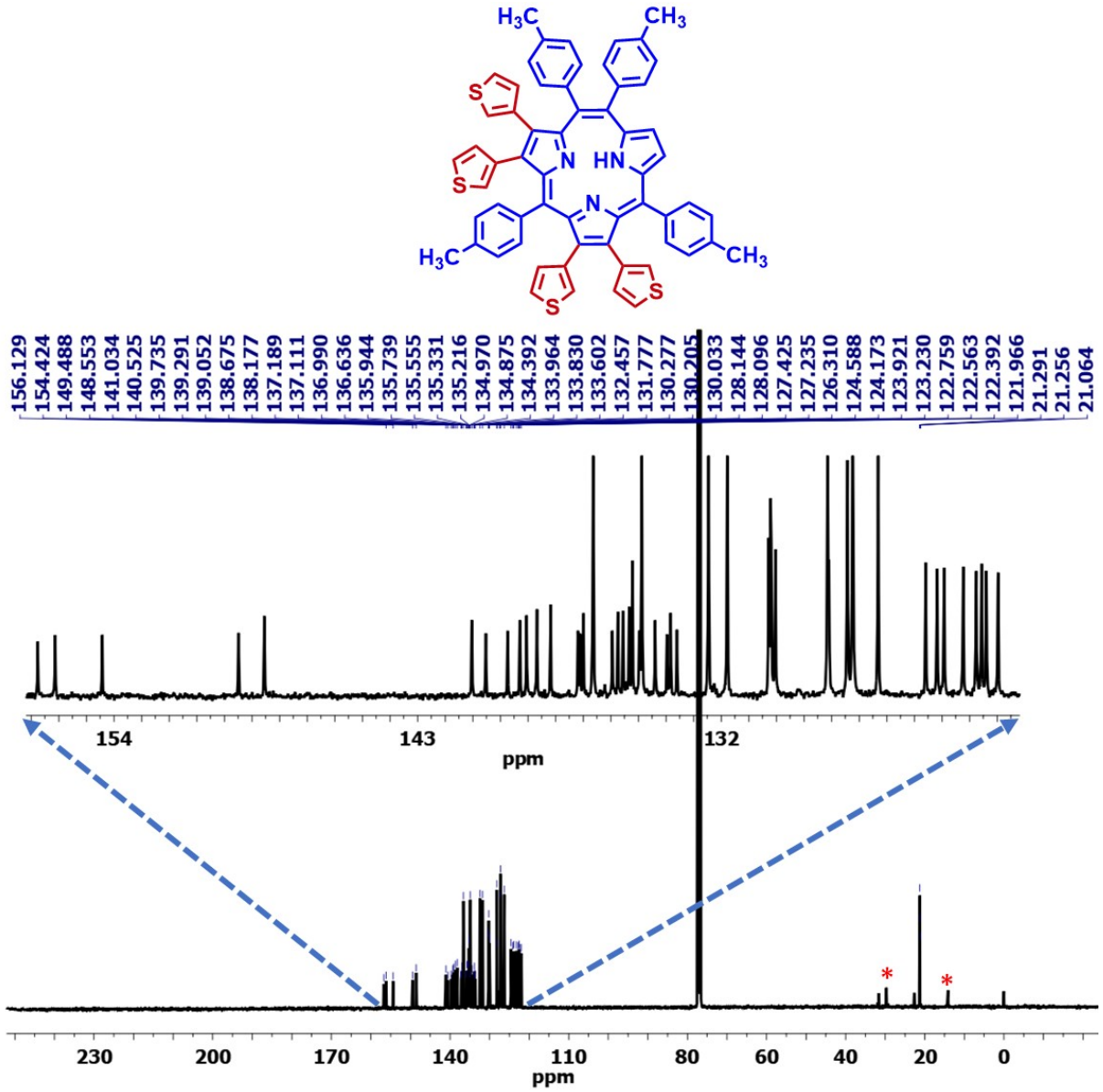

Figure S21. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **14** recorded in $CDCl_3$ on 101 MHz FT-NMR spectrometer. Note: Peaks marked with asterisk (*) are due to residual solvents.

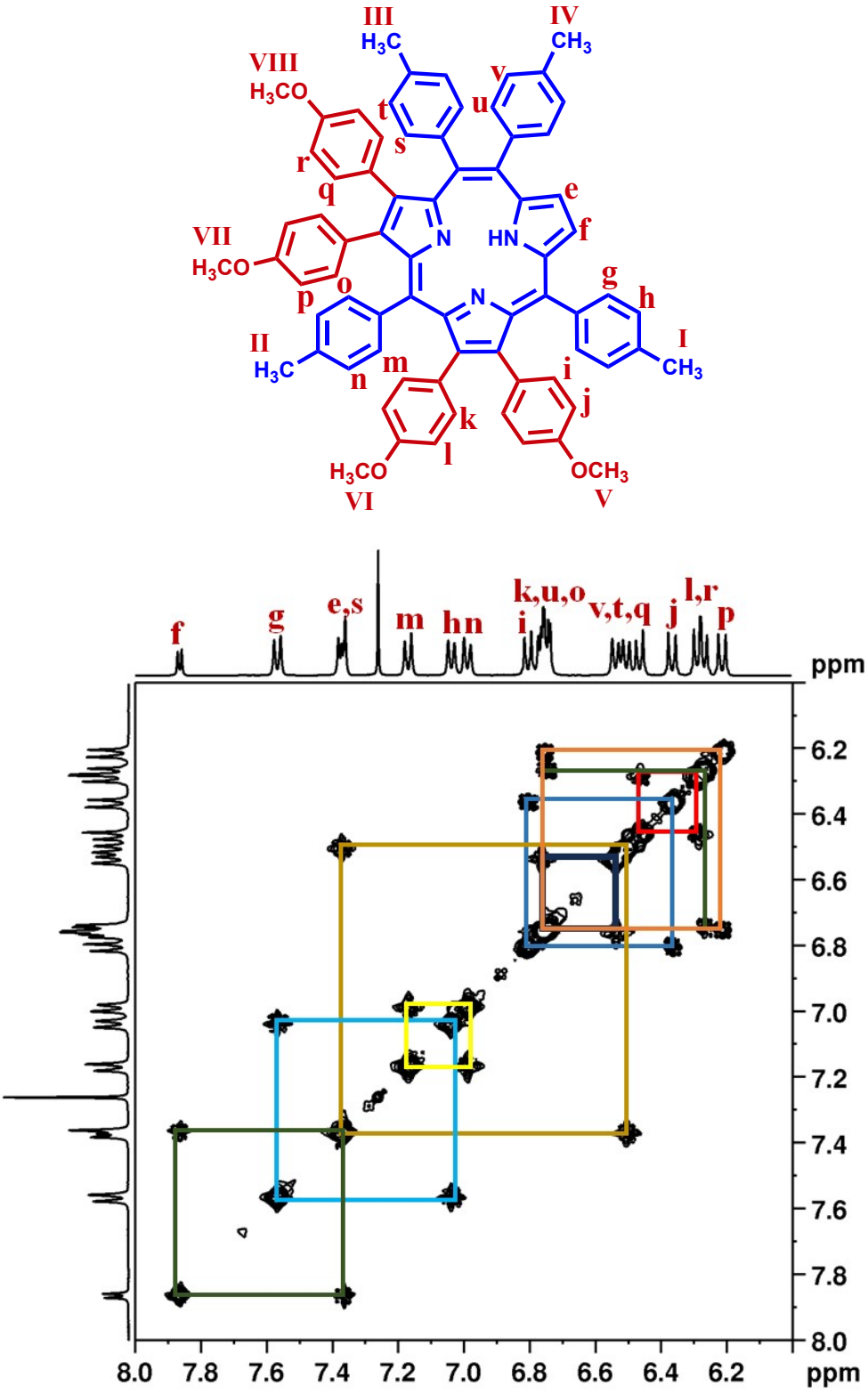

Figure S23. Partial ^{1}H-^{1}H COSY spectrum of compound **12** recorded in $CDCl_3$ at room temperature on 400 MHz instrument.

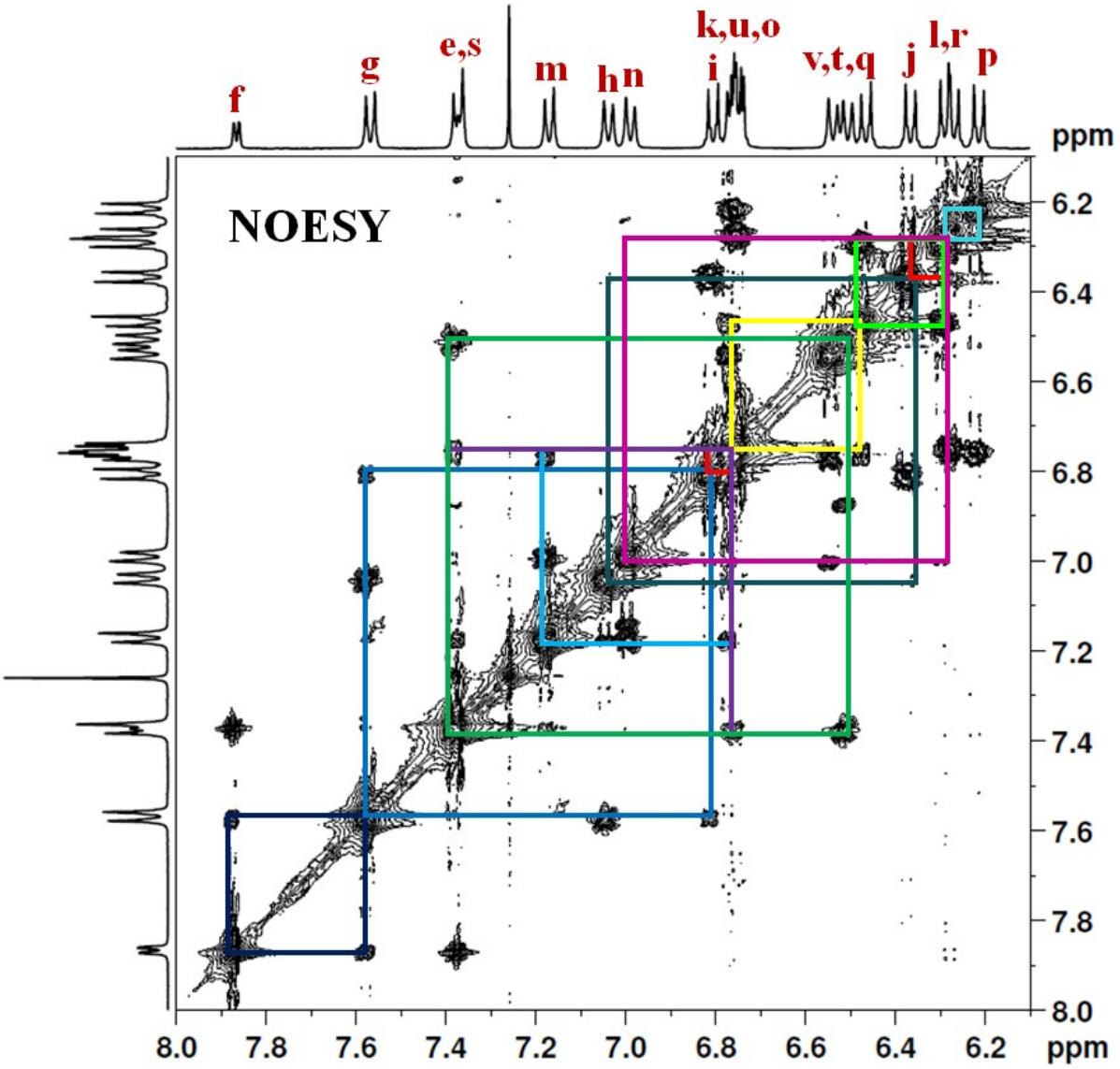

Figure S24. Partial ^{1}H-^{1}H NOESY spectrum of compound **12** recorded in $CDCl_3$ at room temperature on 400 MHz instrument.

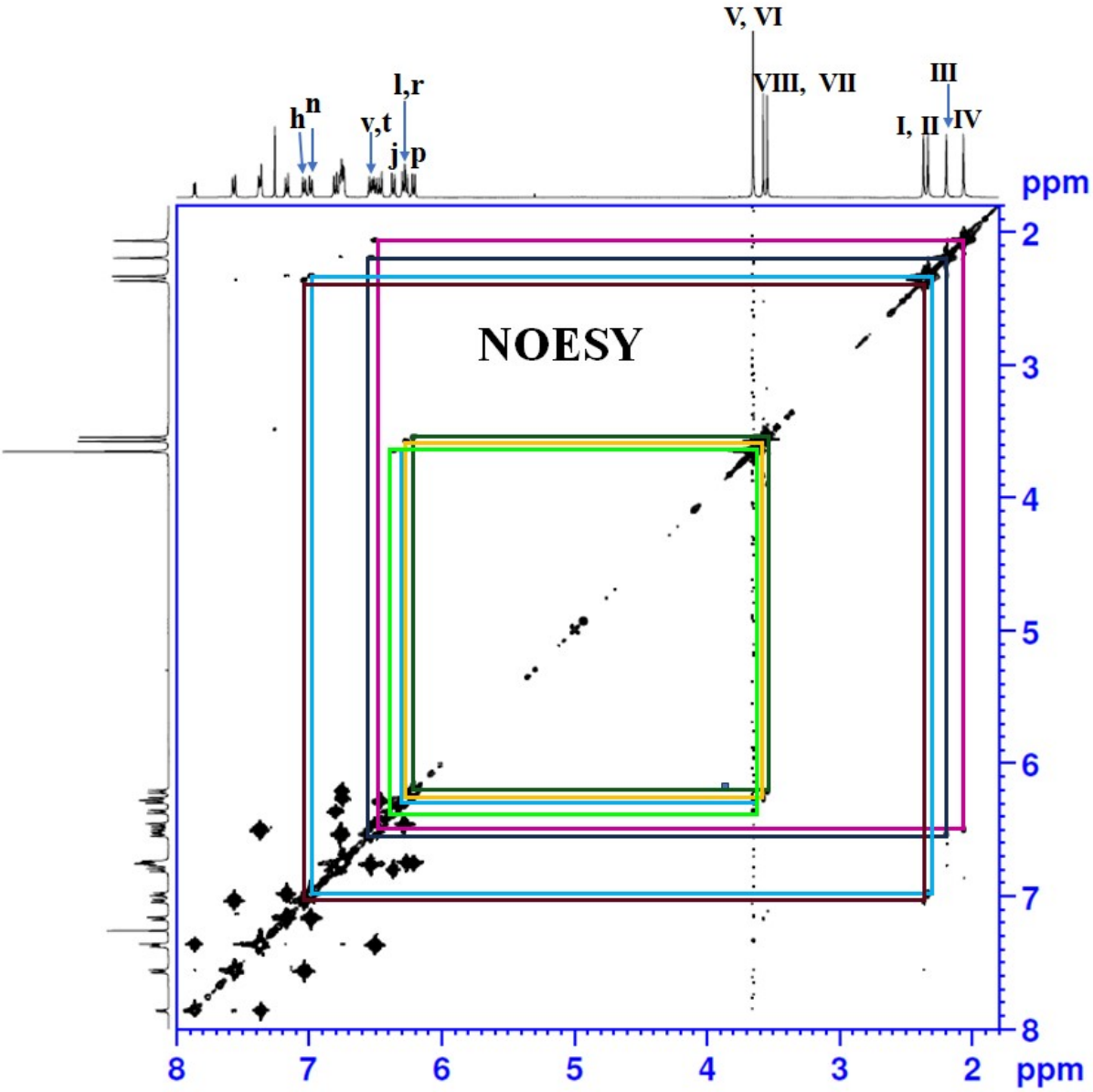

Figure S25. ^{1}H-^{1}H NOESY spectrum of compound **12** recorded in $CDCl_3$ at room temperature on 400 MHz instrument.

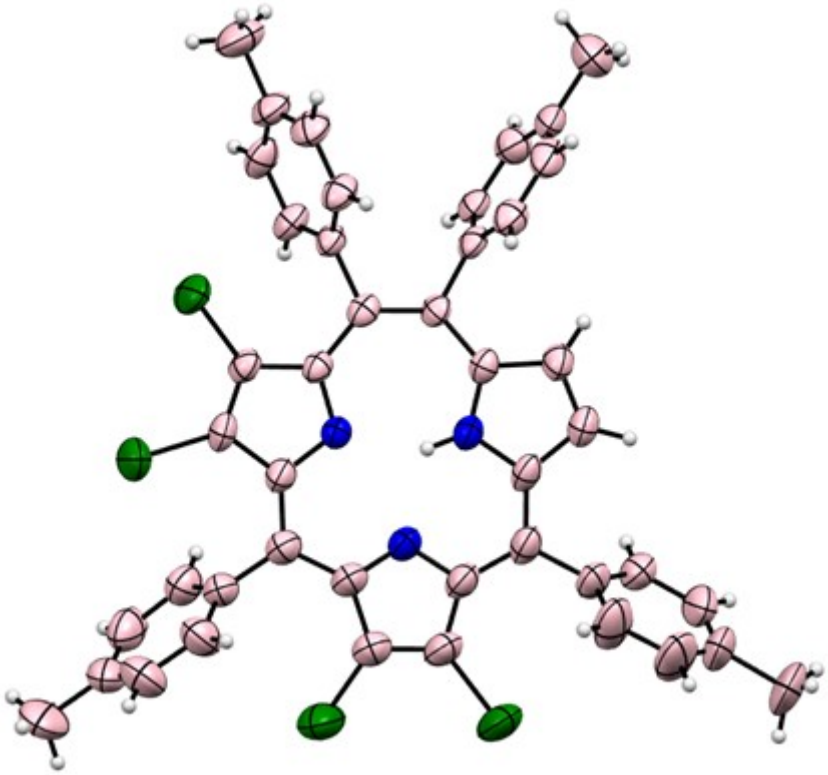

Figure S26. X-ray crystal structure of compound **8**. Thermal Ellipsoids are set at 50% probability.

Table S1. Crystal data and structure refinement for compound **8**.

Identification code	MR-AS-BR4
Empirical formula	$C_{44}H_{31}Br_4N_3$
Formula weight	921.36
Temperature/K	301.00
Crystal system	monoclinic
Space group	C2/c
a/Å	41.29(3)
b/Å	8.552(7)
c/Å	23.83(2)
α/°	90
β/°	113.027(16)
γ/°	90
Volume/Å^3	7746(12)
Z	8
ρ_{calc}g/cm^3	1.580
μ/mm^{-1}	4.192
F(000)	3648.0
Crystal size/mm^3	0.25 × 0.201 × 0.013
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.288 to 51.362
Index ranges	-40 ≤ h ≤ 50, -10 ≤ k ≤ 10, -29 ≤ l ≤ 29
Reflections collected	43561
Independent reflections	7330 [R_{int} = 0.1477, R_{sigma} = 0.1152]
Data/restraints/parameters	7330/469/464
Goodness-of-fit on F^2	0.994
Final R indexes [I>=2σ (I)]	R_1 = 0.0586, wR_2 = 0.0970
Final R indexes [all data]	R_1 = 0.1683, wR_2 = 0.1273
Largest diff. peak/hole / e Å^{-3}	0.77/-0.50

Table S2. Bond Lengths for compound **8**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Br1	C2	1.852(7)	C16	C38	1.487(8)
Br2	C3	1.866(7)	C17	C18	1.377(9)
Br3	C7	1.876(6)	C17	C22	1.372(9)
Br4	C8	1.862(6)	C18	C19	1.383(10)
N1	C1	1.350(7)	C19	C20	1.356(11)
N1	C4	1.336(8)	C20	C21	1.385(11)
N2	C6	1.380(7)	C20	C23	1.515(10)
N2	C9	1.351(7)	C21	C22	1.415(10)

N3	C12	1.337(7)	C24	C25	1.390(8)
N3	C15	1.375(7)	C24	C29	1.379(8)
C1	C2	1.446(9)	C25	C26	1.385(8)
C1	C16	1.419(9)	C26	C27	1.380(9)
C2	C3	1.389(9)	C27	C28	1.384(9)
C3	C4	1.476(8)	C27	C30	1.516(8)
C4	C5	1.428(8)	C28	C29	1.377(8)
C5	C6	1.415(8)	C31	C32	1.373(8)
C5	C17	1.489(9)	C31	C36	1.395(8)
C6	C7	1.459(8)	C32	C33	1.402(8)
C7	C8	1.358(8)	C33	C34	1.382(9)
C8	C9	1.467(8)	C34	C35	1.386(9)
C9	C10	1.434(8)	C34	C37	1.529(9)
C10	C11	1.411(8)	C35	C36	1.375(9)
C10	C24	1.507(8)	C38	C39	1.392(9)
C11	C12	1.434(7)	C38	C43	1.394(9)
C11	C31	1.519(8)	C39	C40	1.373(9)
C12	C13	1.439(8)	C40	C41	1.378(12)
C13	C14	1.356(8)	C41	C42	1.363(12)
C14	C15	1.428(8)	C41	C44	1.554(11)
C15	C16	1.414(8)	C42	C43	1.387(10)

Table S3. Bond Angles for compound **8**.

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
C4	N1	C1	109.7(6)	C1	C16	C38	122.9(6)
C9	N2	C6	109.5(5)	C15	C16	C1	120.0(6)
C12	N3	C15	111.6(5)	C15	C16	C38	117.0(6)
N1	C1	C2	109.3(6)	C18	C17	C5	120.8(7)
N1	C1	C16	117.6(6)	C22	C17	C5	120.3(7)
C16	C1	C2	131.9(6)	C22	C17	C18	118.9(7)
C1	C2	Br1	128.7(6)	C17	C18	C19	119.8(8)
C3	C2	Br1	125.0(6)	C20	C19	C18	122.5(9)
C3	C2	C1	106.2(6)	C19	C20	C21	118.4(9)
C2	C3	Br2	124.0(5)	C19	C20	C23	121.4(10)
C2	C3	C4	105.8(6)	C21	C20	C23	120.1(10)
C4	C3	Br2	129.9(5)	C20	C21	C22	119.5(8)
N1	C4	C3	108.6(6)	C17	C22	C21	120.7(8)
N1	C4	C5	119.9(6)	C25	C24	C10	119.8(6)
C5	C4	C3	131.4(7)	C29	C24	C10	122.2(6)
C4	C5	C17	119.7(6)	C29	C24	C25	118.0(6)

C6	C5	C4	118.3(6)	C26	C25	C24	120.0(6)
C6	C5	C17	122.0(6)	C27	C26	C25	122.4(6)
N2	C6	C5	123.9(6)	C26	C27	C28	116.6(6)
N2	C6	C7	107.2(5)	C26	C27	C30	121.7(7)
C5	C6	C7	128.8(6)	C28	C27	C30	121.8(7)
C6	C7	Br3	128.2(5)	C29	C28	C27	121.9(7)
C8	C7	Br3	123.5(5)	C28	C29	C24	121.1(6)
C8	C7	C6	108.0(5)	C32	C31	C11	122.0(6)
C7	C8	Br4	123.4(5)	C32	C31	C36	118.8(6)
C7	C8	C9	106.6(5)	C36	C31	C11	119.1(6)
C9	C8	Br4	129.4(5)	C31	C32	C33	120.4(6)
N2	C9	C8	108.5(5)	C34	C33	C32	120.6(7)
N2	C9	C10	122.9(5)	C33	C34	C35	118.4(7)
C10	C9	C8	128.6(6)	C33	C34	C37	120.1(7)
C9	C10	C24	116.0(5)	C35	C34	C37	121.4(7)
C11	C10	C9	129.1(5)	C36	C35	C34	121.0(7)
C11	C10	C24	114.9(5)	C35	C36	C31	120.7(7)
C10	C11	C12	130.5(6)	C39	C38	C16	122.1(6)
C10	C11	C31	118.4(5)	C39	C38	C43	118.8(7)
C12	C11	C31	111.1(5)	C43	C38	C16	119.2(7)
N3	C12	C11	126.2(6)	C40	C39	C38	120.4(7)
N3	C12	C13	106.3(5)	C39	C40	C41	121.0(9)
C11	C12	C13	127.5(6)	C40	C41	C44	120.3(11)
C14	C13	C12	108.3(6)	C42	C41	C40	118.9(8)
C13	C14	C15	107.7(6)	C42	C41	C44	120.8(10)
N3	C15	C14	106.0(6)	C41	C42	C43	121.6(9)
N3	C15	C16	124.2(6)	C42	C43	C38	119.3(8)
C16	C15	C14	129.7(6)				

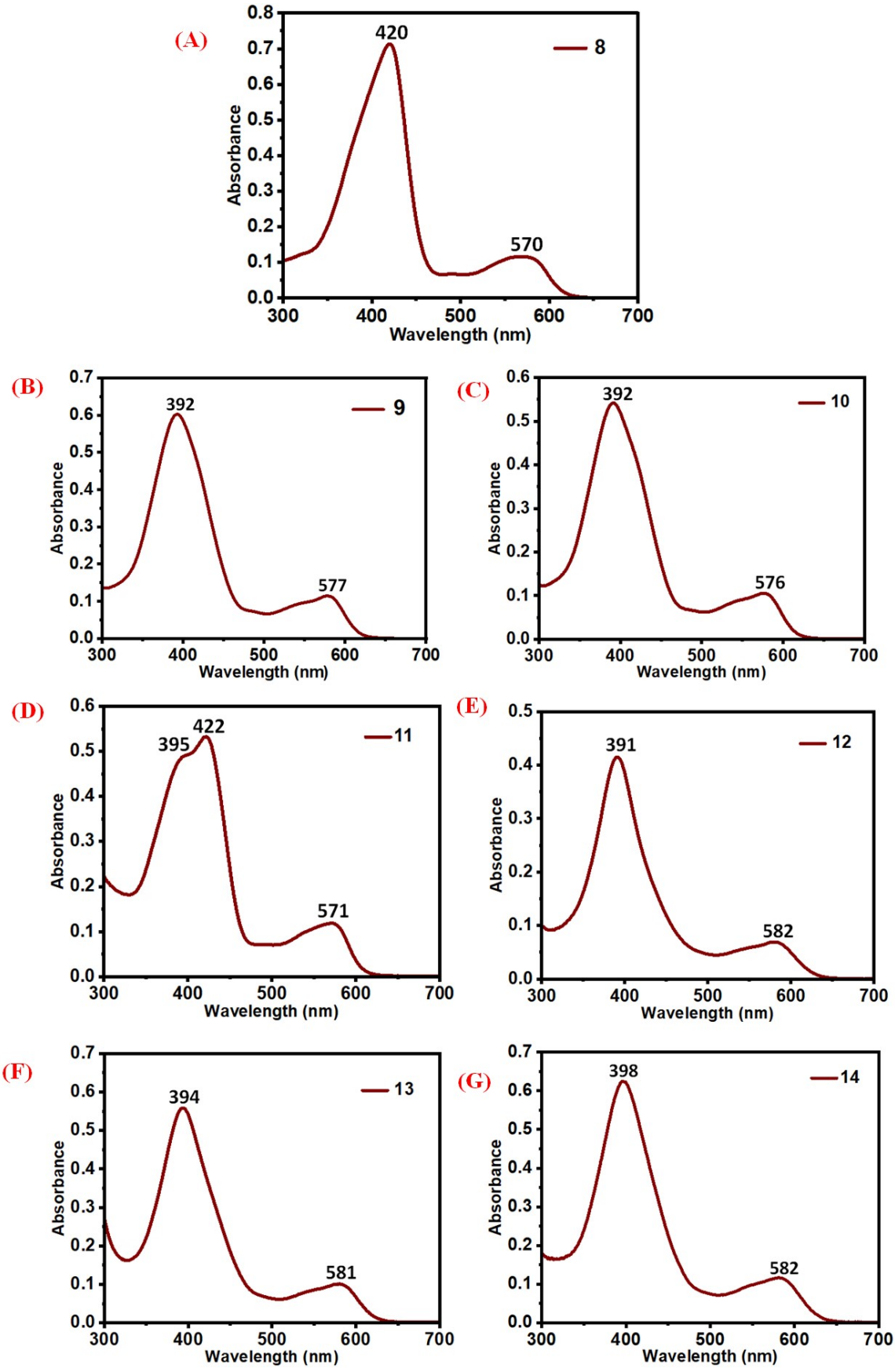

Figure S27. Absorption spectra of compound **8** (A), **9** (B), **10** (C), **11** (D), **12** (E), **13** (F) and **14** (G) (10^{-5} M) recorded in chloroform at room temperature.

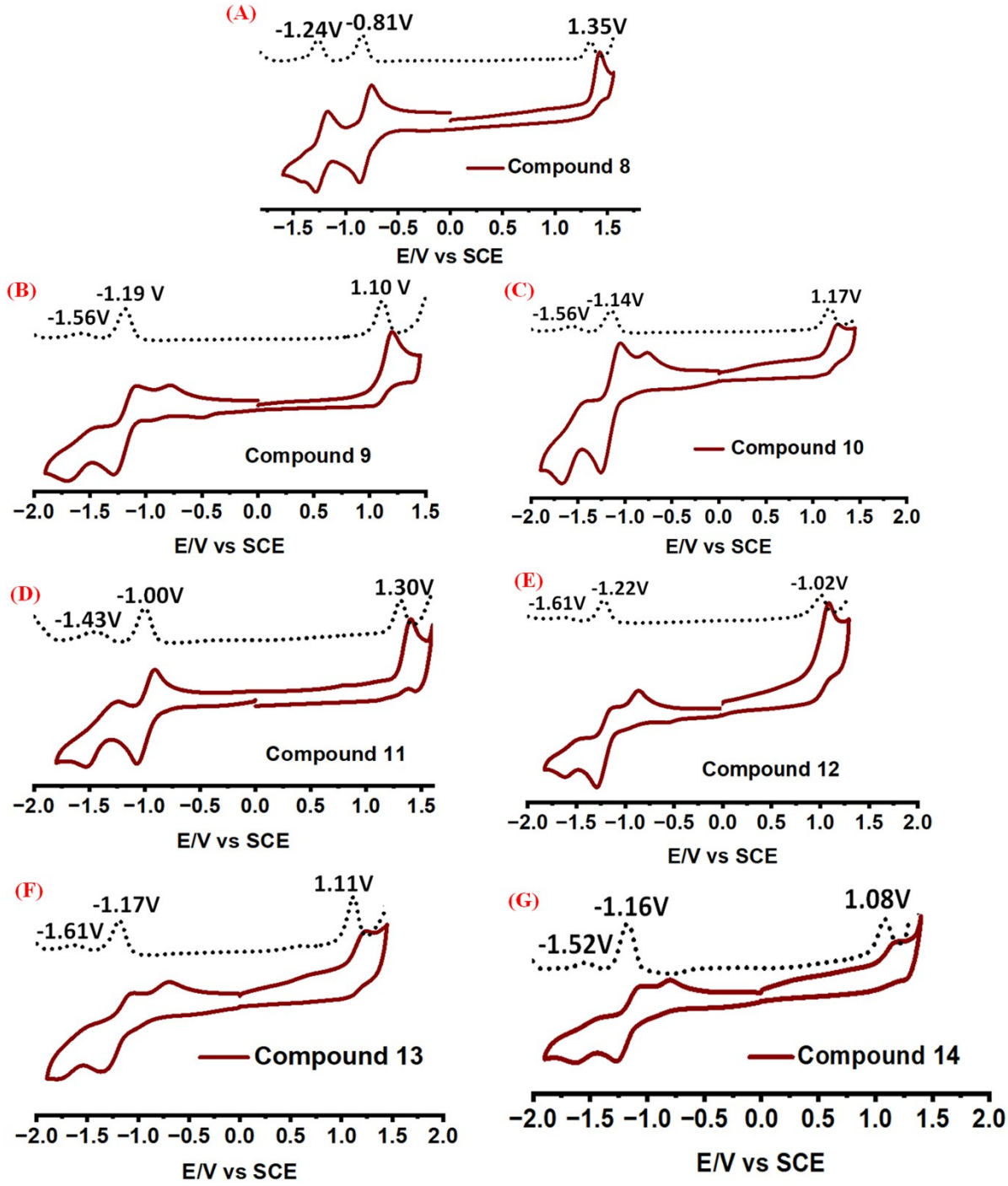

Figure S28. Comparison of cyclic voltammograms (coloured solid line) with their differential pulse voltammogram (dotted black line) of compounds **8-14** recorded in dry CH_2Cl_2 with 0.1 M TBAP as the supporting electrolyte and a saturated calomel electrode (SCE) as the reference electrode at a scan rate of 50 mV s^{-1}. 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)

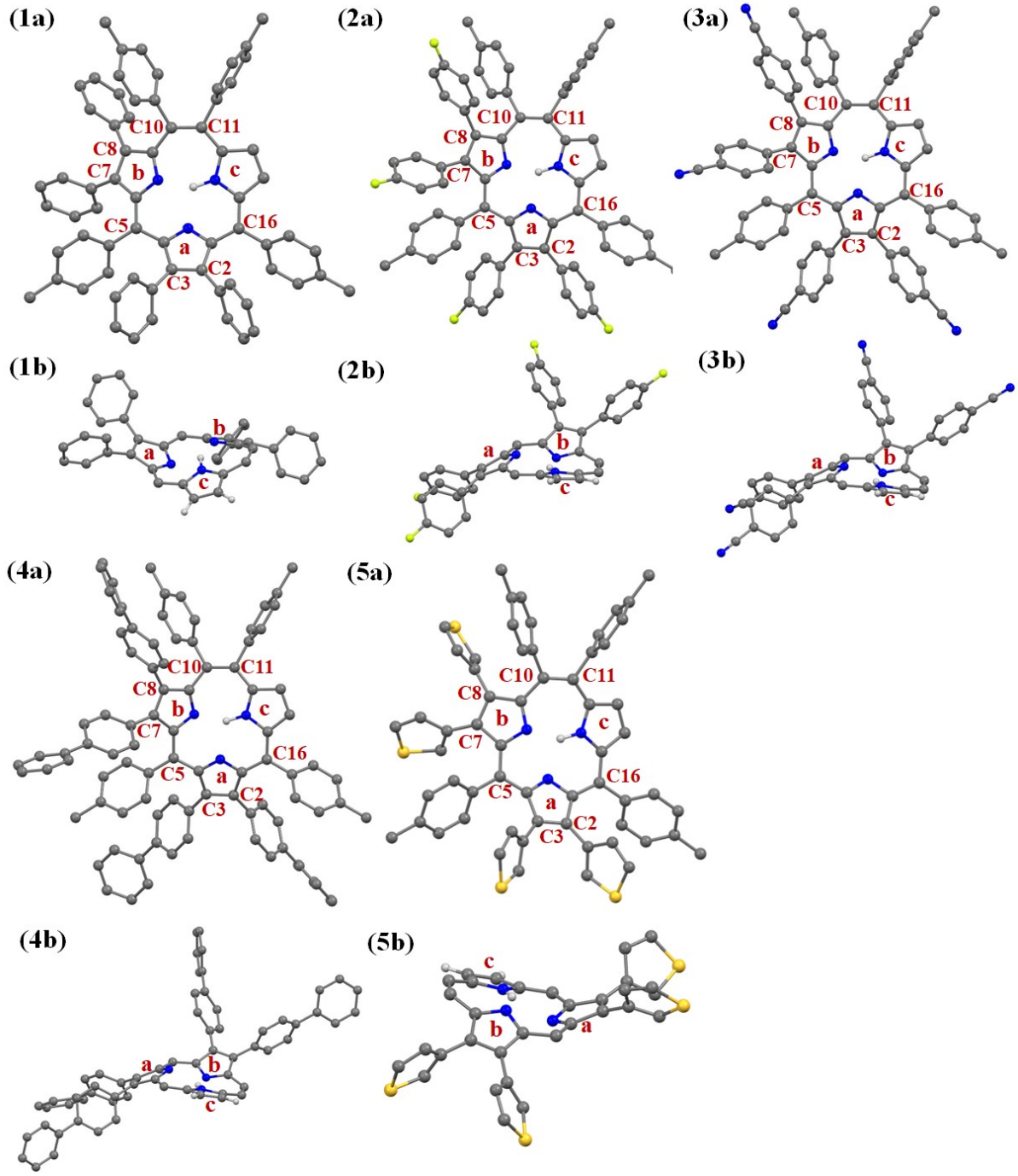

Figure S29. Ground state optimized structures with top views and side views of compounds **9** (1a and 1b), **10** (2a and 2b), **11** (3a and 3b), **13** (4a and 4b), and **14** (5a and 5b).

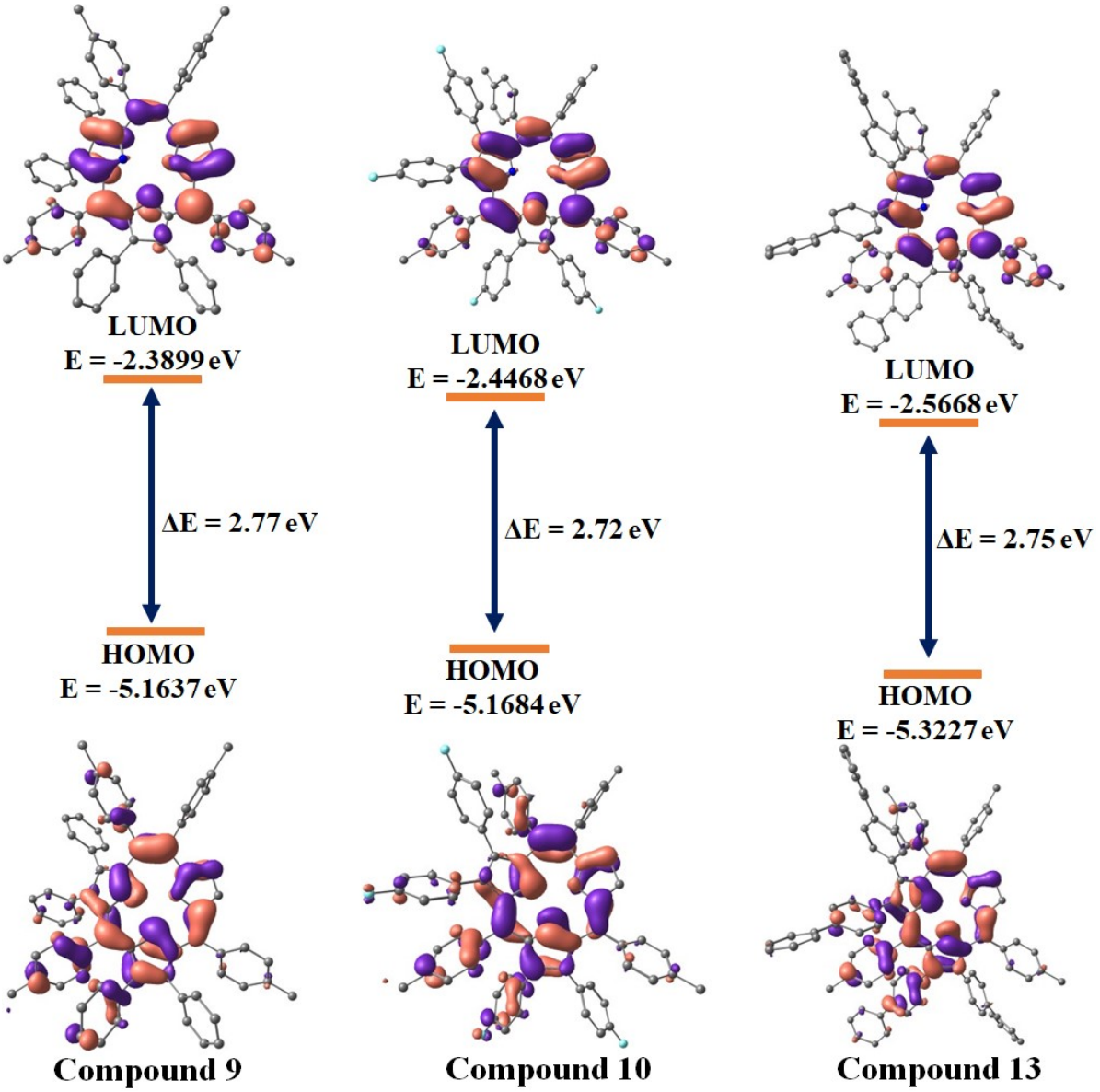

Figure S30. Energy-level diagram (selected FMOs) of compounds **9**, **10** and **13** calculated by B3LYP/6-31G (d, p) method.

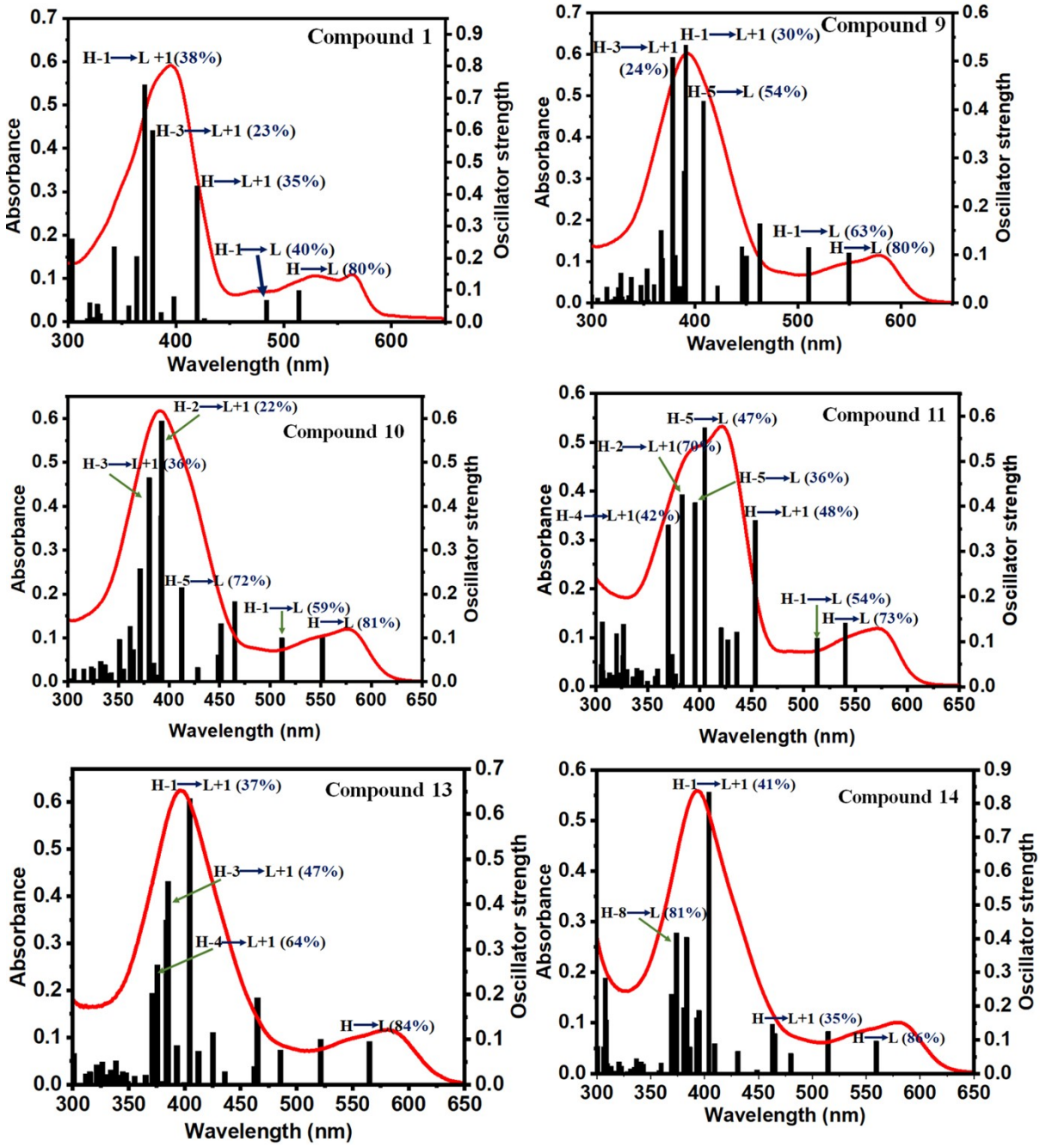

Figure S31. Calculated excitations (black vertical lines) and experimental absorption spectrum (red line) for compounds.

Table S4. Selected TD-DFT calculated oscillator strengths and compositions of the major electronic transitions of **8**.

Wavelength (nm)	Osc. Strength	Major contributions	Minor contributions
537.705755105	0.1443	H-1->LUMO (10%), HOMO->LUMO (72%)	H-1->L+1 (9%), HOMO->L+1 (5%)
509.971178892	0.0724	H-1->LUMO (53%), HOMO->LUMO (14%), HOMO->L+1 (30%)	
465.703312971	0.0641	H-3->LUMO (61%), HOMO->L+1 (21%)	H-2->LUMO (4%), H-1->LUMO (8%)
453.059245093	0.0322	H-4->LUMO (12%), H-2->LUMO (83%)	HOMO->L+1 (3%)
440.989482526	0.116	H-4->LUMO (63%), H-1->L+1 (14%)	H-3->LUMO (3%), H-2->LUMO (6%), H-1->LUMO (3%), HOMO->L+1 (5%)
435.215504817	0.3099	H-4->LUMO (12%), H-3->LUMO (29%), H-1->LUMO (16%), HOMO->L+1 (20%)	H-5->LUMO (3%), H-4->L+1 (5%), H-2->LUMO (4%), H-2->L+1 (6%)
410.353455392	0.2689	H-5->LUMO (44%), H-1->L+1 (33%)	H-4->LUMO (6%), H-4->L+1 (4%), HOMO->LUMO (3%)
402.089161707	0.1463	H-5->LUMO (28%), H-3->L+1 (52%), H-1->L+1 (10%)	
399.575213549	0.1391	H-2->L+1 (77%)	H-6->LUMO (2%), H-5->LUMO (3%), H-1->LUMO (2%), HOMO->L+1 (9%)
390.353859997	0.3555	H-5->LUMO (15%), H-3->L+1 (37%)	H-12->LUMO (3%), H-11->LUMO (3%), H-10->LUMO (9%), H-9->LUMO (8%), H-6->LUMO (2%), H-2->L+1 (6%), H-1->L+1 (8%)
385.451075708	0.4671	H-11->LUMO (12%), H-10->LUMO (10%), H-4->L+1 (28%), H-1->L+1 (14%)	H-12->LUMO (4%), H-9->LUMO (7%), H-7->LUMO (3%), H-6->LUMO (7%), H-3->L+1 (3%), HOMO->LUMO (4%)
384.435189644	0.1945	H-11->LUMO (12%), H-10->LUMO (11%), H-9->LUMO (12%), H-6->LUMO (11%), H-4->L+1 (42%)	H-2->L+1 (5%)
382.584605216	0.1209	H-6->LUMO (75%), H-4->L+1 (16%)	
365.336337956	0.013	H-7->LUMO (55%), H-5->L+1 (29%)	H-9->LUMO (4%), H-8->LUMO (6%)
364.777407432	0.0207	H-8->LUMO (86%)	H-8->L+1 (3%), H-7->LUMO (3%), H-5->L+1 (3%)
360.702275077	0.1072	H-7->LUMO (31%), H-5->L+1 (55%)	H-10->LUMO (3%)

353.846265625	0.0308	H-11->LUMO (31%), H-9->LUMO (53%)	H-12->LUMO (2%), H-10->LUMO (3%), H-5->L+1 (4%)
352.448101121	0.0084	H-11->LUMO (25%), H-10->LUMO (53%), H-9->LUMO (10%)	H-10->L+1 (5%), H-9->L+1 (3%)
348.319126316	0.067	H-11->L+1 (29%), H-10->L+1 (24%), H-9->L+1 (20%)	H-13->L+1 (3%), H-11->LUMO (6%), H-7->L+1 (5%)
342.545083609	0.0023	H-6->L+1 (85%)	H-12->LUMO (7%)
336.858645363	0.0686	H-13->LUMO (68%), H-12->LUMO (14%)	H-6->L+1 (7%)
330.703883631	0.1065	H-13->LUMO (13%), H-12->LUMO (39%), H-8->L+1 (24%)	H-15->LUMO (4%), H-7->L+1 (6%), H-6->L+1 (3%), H-1->L+1 (2%)
330.483508402	0.0632	H-12->LUMO (10%), H-8->L+1 (66%)	H-13->LUMO (6%), H-8->LUMO (3%), H-7->L+1 (6%)
325.127689233	0.016	H-15->LUMO (15%), H-7->L+1 (62%)	H-14->LUMO (5%), H-12->LUMO (4%), H-10->L+1 (2%), H-9->L+1 (2%)
321.635864409	0.1205	H-15->LUMO (55%), H-14->LUMO (10%), H-7->L+1 (16%)	H-13->LUMO (4%), H-12->LUMO (7%)
317.322361313	0.0182	H-10->L+1 (21%), H-9->L+1 (67%)	H-11->L+1 (8%)
313.020255528	0.0058	H-11->L+1 (53%), H-10->L+1 (41%)	
305.778955317	0.0159	H-15->LUMO (14%), H-14->LUMO (78%)	H-15->L+1 (3%)
303.429169654	0.0506	H-12->L+1 (76%)	H-17->LUMO (2%), H-15->L+1 (2%), H-13->L+1 (5%), HOMO->L+2 (7%)
297.52398016	0.035	H-15->L+1 (27%), H-13->L+1 (52%)	H-14->L+1 (5%), H-12->L+1 (9%)
292.836847852	0.0364	H-16->LUMO (63%), H-15->L+1 (14%), H-13->L+1 (14%)	H-14->L+1 (3%)
291.933583735	0.0206	H-16->LUMO (33%), H-15->L+1 (30%), H-13->L+1 (21%)	H-14->L+1 (9%)
287.066897458	0.1465	HOMO->L+2 (84%)	H-12->L+1 (5%)
281.309146009	0.0091	H-17->LUMO (40%), H-1->L+2 (50%)	H-15->L+1 (2%)
276.904953684	0.0036	H-17->LUMO (12%), H-16->L+1 (14%), H-15->L+1 (12%), H-14->L+1 (54%)	H-1->L+2 (2%)
275.839176409	0.0721	H-17->LUMO (33%), H-14->L+1 (17%), H-1->L+2 (34%)	H-16->L+1 (4%), H-15->L+1 (4%)
274.052724326	0.0188	H-16->L+1 (78%)	H-17->LUMO (6%), H-14->L+1 (6%), H-1->L+2 (5%)
262.817579252	0.0183	H-19->LUMO (13%), H-2-	H-18->LUMO (9%), H-4-

		>L+2 (61%)	>L+2 (3%), H-3->L+2 (6%)
261.404581514	0.0034	H-18->LUMO (38%), H-17->L+1 (22%), H-2->L+2 (20%)	H-19->LUMO (9%)
260.94793638	0.0464	H-19->LUMO (46%), H-17->L+1 (19%), H-3->L+2 (26%)	
260.427224442	0.0716	H-19->LUMO (19%), H-18->LUMO (14%), H-3->L+2 (53%)	H-4->L+2 (3%), H-2->L+2 (6%)
256.451811964	0.0479	H-18->LUMO (14%), H-17->L+1 (29%), H-4->L+2 (23%), HOMO->L+4 (11%)	H-19->LUMO (2%), H-3->L+2 (7%), H-2->L+2 (5%)
255.342682701	0.0055	H-4->L+2 (20%), HOMO->L+4 (47%), HOMO->L+5 (11%)	H-6->L+2 (2%), HOMO->L+3 (7%)
254.050351438	0.0169	H-17->L+1 (15%), H-4->L+2 (36%)	H-21->LUMO (3%), H-20->LUMO (9%), H-19->LUMO (4%), H-18->LUMO (8%), HOMO->L+4 (9%)
253.432388317	0.0082	HOMO->L+3 (27%), HOMO->L+4 (13%), HOMO->L+5 (42%)	
251.2497072	0.0181	HOMO->L+3 (38%), HOMO->L+5 (27%)	H-4->L+9 (3%), H-2->L+3 (3%), H-2->L+9 (5%), HOMO->L+9 (8%)
249.646007193	0.0073	H-21->LUMO (14%), H-20->LUMO (55%)	H-18->LUMO (7%), H-17->L+1 (4%), H-4->L+2 (5%)
248.321001847	0.0016	H-3->L+10 (11%), H-1->L+5 (19%), H-1->L+9 (10%)	H-4->L+9 (3%), H-3->L+5 (7%), H-3->L+8 (6%), H-3->L+9 (7%), H-1->L+3 (4%), H-1->L+4 (4%), H-1->L+8 (6%), H-1->L+10 (5%)
248.097396671	0.0095	H-2->L+9 (11%), HOMO->L+3 (10%), HOMO->L+6 (20%), HOMO->L+9 (16%)	H-4->L+9 (6%), H-4->L+10 (3%), H-2->L+6 (2%), H-2->L+10 (3%), HOMO->L+5 (7%), HOMO->L+10 (2%)
245.440350415	0.021	H-21->LUMO (13%), HOMO->L+8 (34%)	H-20->LUMO (7%), H-6->L+2 (4%), H-5->L+2 (4%), H-3->L+5 (2%), H-3->L+9 (2%), HOMO->L+10 (5%), HOMO->L+12 (3%)

Table S5. Selected TD-DFT calculated oscillator strengths and compositions of the major electronic transitions of **9**.

Wavelength (nm)	**Osc. Strength**	**Major contributions**	**Minor contributions**
549.088543013	0.1047	H-1->L+1 (10%), HOMO->LUMO (80%)	H-1->LUMO (5%), HOMO->L+1 (2%)

510.118053949	0.1161	H-1->LUMO (63%), HOMO->L+1 (28%)	HOMO->LUMO (7%)
462.66211289	0.1645	H-3->LUMO (14%), H-2->LUMO (30%), H-1->LUMO (14%), HOMO->L+1 (30%)	H-2->L+1 (5%), H-1->L+1 (3%)
449.674281925	0.0979	H-2->LUMO (37%), H-1->L+1 (20%), HOMO->L+1 (19%)	H-4->LUMO (8%), H-3->LUMO (3%), H-3->L+1 (4%), H-1->LUMO (4%)
445.457525284	0.1172	H-3->LUMO (80%), HOMO->L+1 (10%)	H-1->LUMO (5%)
421.743632261	0.0364	H-4->LUMO (69%), H-2->LUMO (17%)	H-1->L+1 (4%)
408.097801298	0.4179	H-5->LUMO (54%), H-1->L+1 (27%)	H-4->LUMO (2%), H-2->LUMO (3%), HOMO->LUMO (5%)
390.981656246	0.5337	H-7->LUMO (11%), H-5->LUMO (17%), H-4->LUMO (14%), H-3->L+1 (13%), H-1->L+1 (21%)	H-9->LUMO (4%), H-2->LUMO (2%), H-2->L+1 (9%), HOMO->LUMO (4%)
389.165363044	0.2733	H-5->LUMO (13%), H-3->L+1 (39%), H-2->L+1 (30%)	H-2->LUMO (5%), H-1->L+1 (6%)
384.888687835	0.0355	H-9->LUMO (16%), H-7->LUMO (40%), H-5->LUMO (11%), H-2->L+1 (13%)	H-17->LUMO (2%), H-12->LUMO (5%), H-1->L+1 (2%)
380.471332164	0.0998	H-6->LUMO (61%), H-3->L+1 (13%), H-2->L+1 (12%)	H-12->LUMO (3%), H-8->LUMO (2%), H-7->LUMO (2%)
378.035164839	0.5085	H-6->LUMO (17%), H-3->L+1 (24%), H-2->L+1 (22%)	H-15->LUMO (3%), H-13->LUMO (2%), H-11->LUMO (6%), H-8->LUMO (6%), H-5->LUMO (3%), H-1->LUMO (2%), HOMO->L+1 (5%)
368.03666888	0.0937	H-8->LUMO (12%), H-4->L+1 (58%)	H-6->LUMO (8%), H-5->L+1 (8%)
366.871410008	0.1514	H-8->LUMO (58%), H-4->L+1 (17%)	H-12->LUMO (2%), H-7->LUMO (3%), H-6->LUMO (7%)
360.146961634	0.0392	H-9->LUMO (29%), H-7->LUMO (26%), H-5->L+1 (13%)	H-13->LUMO (3%), H-11->LUMO (3%), H-10->LUMO (5%), H-8->LUMO (4%), H-4->L+1 (4%)
354.899650815	0.007	H-11->LUMO (19%), H-9->LUMO (21%), H-5->L+1 (37%)	H-7->LUMO (9%), H-4->L+1 (4%)
353.62423494	0.0718	H-12->LUMO (17%), H-11->LUMO (32%), H-8->LUMO (10%), H-5->L+1 (19%)	H-7->L+1 (4%), H-4->L+1 (5%)
350.336798565	0.0061	H-10->LUMO (89%)	H-11->LUMO (2%), H-9->LUMO (3%)

347.53803227	0.0374	H-12->LUMO (42%), H-11->LUMO (22%), H-9->LUMO (10%)	H-18->LUMO (2%), H-17->LUMO (3%), H-13->LUMO (2%), H-7->LUMO (4%), H-5->L+1 (7%)
341.422572595	0.0052	H-9->L+1 (21%), H-7->L+1 (43%)	H-13->LUMO (2%), H-12->LUMO (5%), H-11->L+1 (3%), H-8->L+1 (5%), H-5->L+1 (5%), H-4->L+1 (2%)
337.84079406	0.0545	H-13->LUMO (70%)	H-14->LUMO (5%), H-11->LUMO (3%), H-9->LUMO (5%), H-7->L+1 (2%), H-5->L+1 (5%)
335.727573821	0.0158	H-17->LUMO (17%), H-15->LUMO (20%), H-14->LUMO (30%)	H-20->LUMO (4%), H-19->LUMO (2%), H-13->LUMO (9%), H-6->L+1 (7%)
333.362532298	0.0025	H-17->LUMO (11%), H-6->L+1 (68%)	H-15->LUMO (5%), H-12->LUMO (3%)
331.313647085	0.007	H-17->LUMO (11%), H-15->LUMO (19%), H-14->LUMO (58%)	H-6->L+1 (6%)
329.053831079	0.0143	H-17->LUMO (33%), H-15->LUMO (35%)	H-18->LUMO (3%), H-16->LUMO (5%), H-12->LUMO (4%), H-8->L+1 (7%), H-6->L+1 (4%)
328.0612627	0.0628	H-16->LUMO (77%)	H-20->LUMO (4%), H-19->LUMO (6%), H-8->L+1 (3%)
327.636470092	0.0077	H-8->L+1 (45%), H-7->L+1 (16%)	H-18->LUMO (7%), H-17->LUMO (6%), H-16->LUMO (2%), H-15->LUMO (5%), H-11->L+1 (5%), H-9->L+1 (3%)
325.622946245	0.0322	H-20->LUMO (15%), H-19->LUMO (52%)	H-21->LUMO (3%), H-16->LUMO (7%), H-15->LUMO (3%), H-14->LUMO (3%)
322.791442365	0.0139	H-18->LUMO (73%)	H-19->LUMO (3%), H-17->LUMO (7%), H-15->LUMO (2%), H-8->L+1 (3%)
320.687478693	0.0089	H-12->L+1 (11%), H-9->L+1 (29%), H-8->L+1 (16%), H-7->L+1 (24%)	H-11->L+1 (3%), H-10->L+1 (4%)
316.100739393	0.0071	H-20->LUMO (49%), H-19->LUMO (27%)	H-21->LUMO (2%), H-12->L+1 (2%), H-11->L+1 (8%), H-8->L+1 (2%)
314.098733342	0.0333	H-20->LUMO (13%), H-12->L+1 (17%), H-11->L+1 (43%)	H-21->LUMO (3%), H-13->L+1 (3%), H-8->L+1 (7%)
311.800103139	0.0037	H-12->L+1 (29%), H-11->L+1 (20%), H-10->L+1 (33%)	H-9->L+1 (8%)

310.72175082	0.003	H-12->L+1 (11%), H-10->L+1 (52%), H-9->L+1 (21%)	H-17->L+1 (3%), H-8->L+1 (4%)
305.455020971	0.0106	H-14->L+1 (10%), H-13->L+1 (62%)	H-17->L+1 (5%), H-15->L+1 (4%), H-11->L+1 (5%), H-9->L+1 (3%), HOMO->L+2 (4%)
299.710387285	0.018	H-17->L+1 (13%), H-15->L+1 (33%), H-13->L+1 (17%)	H-21->LUMO (5%), H-14->L+1 (6%), H-12->L+1 (7%), H-1->L+2 (3%), HOMO->L+2 (8%)
299.204095304	0.0179	H-21->LUMO (14%), H-17->L+1 (12%), H-16->L+1 (32%), H-14->L+1 (13%), HOMO->L+2 (11%)	H-15->L+1 (9%)
297.039274107	0.0736	H-17->L+1 (16%), H-14->L+1 (18%), HOMO->L+2 (32%)	H-18->L+1 (6%), H-16->L+1 (9%), H-15->L+1 (2%), H-13->L+1 (2%), H-12->L+1 (4%), H-1->L+2 (2%)
296.364749641	0.0623	H-21->LUMO (11%), H-16->L+1 (14%), H-14->L+1 (46%), HOMO->L+2 (16%)	H-13->L+1 (3%), H-1->L+2 (5%)
294.905553999	0.0233	H-18->L+1 (14%), H-16->L+1 (17%), H-15->L+1 (30%), HOMO->L+2 (19%)	H-19->L+1 (2%), H-17->L+1 (5%), H-12->L+1 (3%), H-1->L+2 (3%)
294.087129705	0.0416	H-21->LUMO (13%), H-16->L+1 (15%), H-1->L+2 (49%)	H-20->L+1 (4%), H-17->L+1 (5%), HOMO->L+2 (3%)
292.850681466	0.0164	H-18->L+1 (53%), H-17->L+1 (10%)	H-22->LUMO (4%), H-21->LUMO (7%), H-19->L+1 (5%), H-16->L+1 (5%), H-15->L+1 (7%)
290.333910201	0.0888	H-22->LUMO (12%), H-21->LUMO (32%), H-17->L+1 (20%), H-1->L+2 (13%)	H-20->LUMO (3%), H-20->L+1 (3%), H-19->L+1 (5%), H-15->L+1 (3%)
287.793210492	0.0698	H-22->LUMO (20%), H-20->L+1 (11%), H-19->L+1 (28%), H-1->L+2 (18%)	H-21->LUMO (5%), H-20->LUMO (2%), H-18->L+1 (4%)
286.688540274	0.0272	H-22->LUMO (46%), H-19->L+1 (36%)	H-19->LUMO (2%), H-18->L+1 (9%)
280.431088872	0.0163	H-20->L+1 (70%), H-19->L+1 (14%)	H-22->LUMO (6%)
271.680675371	0.0198	HOMO->L+3 (83%)	H-21->L+1 (2%), HOMO->L+4 (7%)
269.648092676	0.0138	H-23->LUMO (51%), H-21->L+1 (35%)	HOMO->L+3 (4%)
267.784434152	0.016	H-21->L+1 (10%), HOMO->L+4 (70%)	H-1->L+4 (3%), HOMO->L+3 (4%)
267.328301628	0.0488	H-23->LUMO (23%), H-21->L+1 (20%), H-1->L+3 (17%), HOMO->L+4 (10%)	H-22->L+1 (4%), H-2->L+2 (6%), HOMO->L+3 (2%), HOMO->L+5 (2%)

Table S6. Selected TD-DFT calculated oscillator strengths and compositions of the major electronic transitions of **10**.

Wavelength (nm)	Osc. Strength	Major contributions	Minor contributions
551.531107706	0.1065	HOMO->LUMO (81%)	H-1->LUMO (5%), H-1->L+1 (9%)
511.507046546	0.1001	H-1->LUMO (59%), HOMO->L+1 (32%)	HOMO->LUMO (6%)
465.004661937	0.1823	H-2->LUMO (34%), H-1->LUMO (17%), HOMO->L+1 (29%)	H-3->LUMO (8%), H-2->L+1 (4%), H-1->L+1 (2%)
451.426153331	0.133	H-2->LUMO (33%), H-1->L+1 (20%), HOMO->L+1 (22%)	H-4->LUMO (7%), H-3->L+1 (5%), H-1->LUMO (6%)
448.357115005	0.0618	H-3->LUMO (87%)	H-1->LUMO (3%), HOMO->L+1 (4%)
428.270096761	0.033	H-4->LUMO (65%), H-2->LUMO (20%)	H-3->LUMO (3%), H-1->L+1 (7%)
412.400854884	0.2147	H-5->LUMO (72%), H-1->L+1 (16%)	H-12->LUMO (3%), HOMO->LUMO (3%)
392.877219761	0.5948	H-5->LUMO (11%), H-3->L+1 (18%), H-2->L+1 (22%), H-1->L+1 (19%)	H-6->LUMO (3%), H-4->LUMO (8%), H-2->LUMO (7%), HOMO->LUMO (3%)
392.392293611	0.3789	H-3->L+1 (18%), H-2->L+1 (36%), H-1->L+1 (19%)	H-5->LUMO (6%), H-4->LUMO (9%), HOMO->LUMO (3%)
387.547490036	0.0159	H-6->LUMO (80%)	H-9->LUMO (3%), H-5->LUMO (3%), H-3->L+1 (5%), H-2->L+1 (3%)
384.733423361	0.0426	H-7->LUMO (55%), H-2->L+1 (12%)	H-12->LUMO (6%), H-11->LUMO (2%), H-6->LUMO (3%), H-3->L+1 (8%)
380.319610467	0.4653	H-12->LUMO (12%), H-7->LUMO (11%), H-3->L+1 (36%), H-2->L+1 (16%)	H-9->LUMO (5%), H-8->LUMO (4%), H-5->LUMO (3%), HOMO->L+1 (3%)
371.343575573	0.2581	H-5->L+1 (17%), H-4->L+1 (68%)	H-12->L+1 (3%)
364.595050909	0.0736	H-9->LUMO (19%), H-8->LUMO (22%), H-5->L+1 (27%)	H-12->LUMO (5%), H-7->LUMO (6%), H-6->LUMO (5%), H-4->L+1 (4%), H-2->L+1 (3%)
361.459412298	0.1265	H-8->LUMO (32%), H-5->L+1 (35%), H-4->L+1 (14%)	H-12->LUMO (5%), H-9->LUMO (4%)
355.143630982	0.0296	H-9->LUMO (52%), H-8->LUMO (35%)	H-5->L+1 (3%), H-4->L+1 (2%)
351.090765737	0.0969	H-12->LUMO (30%), H-11-	H-17->LUMO (2%), H-15-

		>LUMO (16%), H-7->LUMO (20%), H-5->L+1 (11%)	>LUMO (3%), H-13->LUMO (4%), H-10->LUMO (3%)
342.924057564	0.0207	H-11->LUMO (40%), H-10->LUMO (23%)	H-15->LUMO (3%), H-14->LUMO (9%), H-13->LUMO (9%), H-12->LUMO (6%)
341.959326509	0.0108	H-7->L+1 (47%)	H-12->LUMO (6%), H-12->L+1 (8%), H-11->LUMO (4%), H-9->LUMO (2%), H-9->L+1 (4%), H-8->L+1 (9%), H-6->L+1 (7%), H-4->L+1 (2%)
341.394369062	0.0193	H-11->LUMO (20%), H-10->LUMO (46%), H-6->L+1 (24%)	H-9->LUMO (3%)
338.939838743	0.0041	H-10->LUMO (23%), H-6->L+1 (51%)	H-15->LUMO (4%), H-11->LUMO (4%), H-9->LUMO (2%), H-7->L+1 (5%)
336.675699267	0.0388	H-15->LUMO (15%), H-13->LUMO (34%), H-12->LUMO (15%)	H-14->LUMO (5%), H-12->L+1 (3%), H-11->LUMO (3%), H-9->LUMO (2%), H-7->L+1 (8%), H-6->L+1 (7%)
333.479095759	0.0042	H-15->LUMO (29%), H-14->LUMO (12%), H-13->LUMO (43%)	H-18->LUMO (2%), H-16->LUMO (3%)
332.611312942	0.0465	H-15->LUMO (24%), H-14->LUMO (63%)	H-11->LUMO (3%)
328.765891526	0.0061	H-16->LUMO (59%)	H-20->LUMO (9%), H-18->LUMO (9%), H-15->LUMO (5%), H-8->L+1 (2%)
325.187381678	0.0301	H-16->LUMO (12%), H-9->L+1 (14%), H-8->L+1 (39%), H-7->L+1 (11%)	H-20->LUMO (4%), H-19->LUMO (3%), H-11->LUMO (2%), H-6->L+1 (3%)
323.203756451	0.0341	H-20->LUMO (18%), H-19->LUMO (11%), H-18->LUMO (16%), H-16->LUMO (16%), H-8->L+1 (15%)	H-21->LUMO (4%), H-17->LUMO (8%), H-7->L+1 (5%)
320.52167161	0.0029	H-17->LUMO (64%)	H-19->LUMO (2%), H-18->LUMO (5%), H-15->LUMO (7%), H-12->L+1 (8%), H-9->L+1 (2%)
316.625448215	0.0035	H-17->LUMO (11%), H-12->L+1 (24%), H-9->L+1 (23%), H-8->L+1 (19%)	H-18->LUMO (4%), H-7->L+1 (6%)
315.7947913	0.0292	H-12->L+1 (18%), H-9->L+1 (39%)	H-20->LUMO (2%), H-15->L+1 (4%), H-13->L+1 (6%), H-11->L+1 (4%), H-8->L+1 (6%), H-7->L+1 (5%)
314.872493428	0.0023	H-20->LUMO (14%), H-19-	H-17->LUMO (3%)

		>LUMO (17%), H-18->LUMO (53%)	
309.503964183	0.003	H-20->LUMO (33%), H-19->LUMO (55%)	
306.118692934	0.029	H-11->L+1 (23%), H-10->L+1 (60%)	H-14->L+1 (5%)
304.382670101	0.0072	H-15->L+1 (17%), H-12->L+1 (12%), H-11->L+1 (21%), H-10->L+1 (16%)	H-21->LUMO (4%), H-16->L+1 (5%), H-14->L+1 (4%), H-13->L+1 (3%), H-9->L+1 (8%), HOMO->L+2 (3%)
303.317822224	0.0063	H-15->L+1 (19%), H-14->L+1 (11%), H-11->L+1 (39%), H-10->L+1 (11%)	H-21->LUMO (2%), H-13->L+1 (8%)
301.283517234	0.0063	H-15->L+1 (30%), H-14->L+1 (45%)	H-21->LUMO (8%), H-16->L+1 (3%), H-13->L+1 (2%), H-10->L+1 (5%)
299.442562522	0.0049	H-14->L+1 (15%), H-13->L+1 (64%)	H-16->L+1 (2%), H-15->L+1 (6%), H-12->L+1 (6%)
297.745474442	0.0795	H-21->LUMO (30%), H-16->L+1 (10%), HOMO->L+2 (33%)	H-15->L+1 (2%), H-14->L+1 (2%), H-13->L+1 (4%), H-1->L+2 (8%)
295.813215499	0.101	H-21->LUMO (11%), HOMO->L+2 (54%)	H-17->L+1 (7%), H-16->L+1 (8%), H-14->L+1 (5%), H-13->L+1 (4%), H-1->L+2 (3%)
293.808367526	0.0247	H-21->LUMO (16%), H-16->L+1 (53%)	H-20->LUMO (3%), H-17->L+1 (7%), H-15->L+1 (4%), H-14->L+1 (5%), H-12->L+1 (3%), H-1->L+2 (5%)
292.774612761	0.0115	H-22->LUMO (58%), H-1->L+2 (17%)	H-20->L+1 (7%), H-19->L+1 (3%)
290.59249288	0.0142	H-22->LUMO (10%), H-18->L+1 (30%), H-17->L+1 (31%)	H-20->L+1 (3%), H-16->L+1 (5%), H-15->L+1 (7%), H-1->L+2 (5%)
288.295105363	0.156	H-22->LUMO (14%), H-21->LUMO (10%), H-1->L+2 (49%)	H-20->LUMO (3%), H-18->L+1 (3%), H-17->L+1 (5%)
286.496425299	0.0245	H-19->L+1 (13%), H-18->L+1 (30%), H-17->L+1 (28%)	H-22->LUMO (3%), H-20->L+1 (9%), H-16->L+1 (4%), H-1->L+2 (6%)
282.920368328	0.0051	H-19->L+1 (49%), H-18->L+1 (18%), H-17->L+1 (10%)	H-21->L+1 (2%), H-20->L+1 (9%), H-12->L+1 (2%)
279.099099593	0.0049	H-20->L+1 (58%), H-19->L+1 (26%)	H-18->L+1 (7%)
274.933903256	0.0236	HOMO->L+3 (89%)	H-3->L+3 (2%), H-1->L+3 (2%)
272.63654018	0.0118	HOMO->L+4 (82%)	H-21->L+1 (8%)
270.755138479	0.037	H-23->LUMO (16%), H-21->L+1 (54%)	H-22->L+1 (3%), H-20->L+1 (5%), HOMO->L+3 (2%), HOMO->L+4 (7%), HOMO-

			>L+5 (3%)
269.595322821	0.0203	H-23->LUMO (13%), H-1->L+3 (21%), HOMO->L+5 (56%)	

Table S7. Selected TD-DFT calculated oscillator strengths and compositions of the major electronic transitions of **11**.

Wavelength (nm)	Osc. Strength	Major contributions	Minor contributions
540.259675856	0.1413	H-1->L+1 (10%), HOMO->LUMO (73%)	H-1->LUMO (9%), HOMO->L+1 (5%)
513.15836684	0.1078	H-1->LUMO (54%), HOMO->LUMO (13%), HOMO->L+1 (30%)	
453.490098801	0.3695	H-2->LUMO (11%), H-1->LUMO (24%), HOMO->L+1 (48%)	H-4->L+1 (4%), H-3->LUMO (6%), H-2->L+1 (3%)
435.827450127	0.1217	H-3->LUMO (17%), H-2->LUMO (33%), H-1->L+1 (25%)	H-5->LUMO (5%), H-4->LUMO (8%), H-4->L+1 (3%), HOMO->L+1 (4%)
427.384326137	0.104	H-3->LUMO (31%), H-2->LUMO (45%), H-1->L+1 (16%)	H-4->LUMO (4%)
420.856052316	0.1308	H-4->LUMO (71%)	H-3->LUMO (5%), H-2->LUMO (8%), H-1->LUMO (3%), H-1->L+1 (4%), HOMO->L+1 (3%)
404.952127943	0.5744	H-5->LUMO (47%), H-1->L+1 (23%)	H-12->LUMO (4%), H-4->LUMO (5%), H-3->LUMO (4%), HOMO->LUMO (6%)
395.761596694	0.4085	H-5->LUMO (36%), H-3->LUMO (27%), H-1->L+1 (12%)	H-6->LUMO (4%), H-4->LUMO (7%), H-2->L+1 (7%), HOMO->LUMO (2%), HOMO->L+1 (2%)
383.389075148	0.4262	H-2->L+1 (70%)	H-12->LUMO (3%), H-6->LUMO (5%), H-5->LUMO (4%), H-4->L+1 (3%), H-3->LUMO (3%), H-3->L+1 (3%), H-1->L+1 (2%)
381.93639644	0.0079	H-9->LUMO (17%), H-6->LUMO (48%)	H-12->LUMO (3%), H-11->LUMO (5%), H-10->LUMO (3%), H-8->LUMO (5%), H-7->LUMO (2%), H-5->LUMO (3%), H-2->L+1 (6%)
376.977691667	0.0291	H-9->LUMO (17%), H-6->LUMO (33%), H-4->L+1 (11%), H-3->L+1 (12%)	H-12->LUMO (4%), H-11->LUMO (3%), H-10->LUMO (3%), H-8->LUMO (2%), H-7->LUMO (6%)

373.435116449	0.0721	H-4->L+1 (23%), H-3->L+1 (45%)	H-9->LUMO (9%), H-7->LUMO (4%), H-6->LUMO (5%)
369.980582532	0.3586	H-5->L+1 (11%), H-4->L+1 (42%), H-3->L+1 (22%), H-2->L+1 (10%)	H-12->L+1 (2%), HOMO->L+1 (2%)
359.655942367	0.0402	H-5->L+1 (63%)	H-12->LUMO (4%), H-8->LUMO (2%), H-7->LUMO (7%), H-4->L+1 (5%), H-3->L+1 (8%)
359.426563305	0.003	H-8->LUMO (29%), H-7->LUMO (43%)	H-13->LUMO (5%), H-12->LUMO (3%), H-5->L+1 (9%)
357.529825861	0.0232	H-9->LUMO (24%), H-8->LUMO (41%), H-7->LUMO (27%)	
349.931396269	0.0123	H-11->LUMO (51%), H-10->LUMO (14%), H-9->LUMO (20%)	H-8->LUMO (5%), H-5->L+1 (3%)
349.270925157	0.0045	H-11->LUMO (20%), H-10->LUMO (73%)	H-12->LUMO (3%)
344.24753724	0.0359	H-13->LUMO (23%), H-12->LUMO (16%), H-6->L+1 (17%)	H-18->LUMO (2%), H-16->LUMO (2%), H-11->L+1 (2%), H-9->L+1 (7%), H-8->LUMO (6%), H-8->L+1 (2%), H-7->LUMO (6%), H-3->L+1 (2%)
339.785121577	0.0408	H-12->LUMO (20%), H-9->L+1 (25%)	H-13->LUMO (2%), H-12->L+1 (6%), H-11->LUMO (4%), H-11->L+1 (7%), H-10->L+1 (4%), H-8->L+1 (3%), H-7->L+1 (6%), H-6->L+1 (4%), H-5->L+1 (8%)
339.106703715	0.008	H-13->LUMO (28%), H-6->L+1 (52%)	H-14->LUMO (3%), H-12->LUMO (3%), H-8->LUMO (2%)
336.091604804	0.0219	H-13->LUMO (12%), H-12->LUMO (21%), H-9->L+1 (11%), H-6->L+1 (20%)	H-17->LUMO (3%), H-14->LUMO (8%), H-12->L+1 (3%), H-7->L+1 (3%)
330.333820937	0.039	H-14->LUMO (11%), HOMO->L+2 (36%), HOMO->L+3 (37%)	H-17->LUMO (3%), H-15->LUMO (4%)
327.048781356	0.0436	H-15->LUMO (10%), HOMO->L+3 (22%), HOMO->L+4 (19%)	H-18->LUMO (8%), H-16->LUMO (3%), H-14->LUMO (6%), H-12->LUMO (4%), H-8->L+1 (3%), H-7->L+1 (3%), H-1->L+2 (3%), H-1->L+4 (3%)
326.824633626	0.1394	H-14->LUMO (11%), HOMO->L+2 (24%), HOMO->L+4 (31%)	H-18->LUMO (3%), H-17->LUMO (3%), H-15->LUMO (5%), H-12->LUMO (2%), H-

			1->L+3 (3%), HOMO->L+3 (2%)
326.102559212	0.0692	HOMO->L+2 (31%), HOMO->L+3 (21%), HOMO->L+4 (37%)	HOMO->L+5 (5%)
324.379135085	0.0307	H-9->L+1 (23%), H-8->L+1 (24%), H-7->L+1 (31%)	HOMO->L+3 (9%)
322.623453063	0.0062	H-15->LUMO (10%), H-14->LUMO (26%), H-13->LUMO (14%), H-7->L+1 (12%)	H-18->LUMO (6%), H-16->LUMO (9%), H-8->L+1 (7%), HOMO->L+3 (3%)
320.944818959	0.0082	H-8->L+1 (38%), H-7->L+1 (23%)	H-18->LUMO (3%), H-15->LUMO (8%), H-14->LUMO (8%), H-13->L+1 (6%), HOMO->L+5 (3%)
320.23192141	0.1179	H-1->L+2 (21%), HOMO->L+5 (62%)	H-1->L+4 (4%), HOMO->L+4 (5%)
318.095782159	0.0255	H-1->L+2 (37%), H-1->L+3 (18%), HOMO->L+5 (12%)	H-16->LUMO (6%), H-15->LUMO (2%), H-1->L+4 (7%), H-1->L+5 (4%)
316.552692349	0.0033	H-16->LUMO (11%), H-1->L+3 (44%)	H-15->LUMO (9%), H-12->L+1 (6%), H-10->L+1 (8%), H-7->L+1 (4%), H-1->L+2 (5%)
316.39920638	0.0215	H-16->LUMO (24%), H-15->LUMO (13%), H-1->L+2 (13%), H-1->L+3 (19%)	H-17->LUMO (3%), H-14->LUMO (5%), H-1->L+4 (2%), HOMO->L+5 (9%)
314.544975549	0.004	H-17->LUMO (20%), H-15->LUMO (18%), H-10->L+1 (23%)	H-18->LUMO (4%), H-14->LUMO (2%), H-11->L+1 (8%), H-9->L+1 (7%), H-8->L+1 (4%), H-7->L+1 (2%), H-1->L+3 (3%)
313.884032942	0.0186	H-17->LUMO (13%), H-10->L+1 (21%), H-1->L+4 (27%)	H-19->LUMO (2%), H-18->LUMO (3%), H-16->LUMO (4%), H-15->LUMO (6%), H-14->LUMO (8%), H-9->L+1 (2%), H-1->L+3 (4%)
313.392126314	0.031	H-10->L+1 (21%), H-1->L+4 (46%)	H-17->LUMO (6%), H-15->LUMO (3%), H-13->L+1 (3%), H-1->L+2 (7%)
311.957007378	0.0185	H-18->LUMO (11%), H-11->L+1 (45%), H-10->L+1 (14%)	H-16->LUMO (7%), H-12->L+1 (5%), H-11->LUMO (3%), H-9->L+1 (5%), H-8->L+1 (2%)
310.138812348	0.0041	H-18->LUMO (25%), H-17->LUMO (30%), H-16->LUMO (21%), H-11->L+1 (13%)	H-9->L+1 (2%), H-1->L+5 (2%)
309.650831699	0.018	H-13->L+1 (13%), H-1->L+5	

		(71%)	
307.378503104	0.0363	H-19->LUMO (13%), H-13->L+1 (17%), H-12->L+1 (27%)	H-18->LUMO (9%), H-11->L+1 (3%), H-8->L+1 (3%), H-7->L+1 (2%), H-1->L+5 (6%)
306.37588468	0.1441	H-19->LUMO (12%), H-13->L+1 (29%), H-12->L+1 (15%)	H-14->L+1 (7%), H-11->L+1 (5%), H-8->L+1 (2%), H-1->L+2 (4%), H-1->L+5 (8%)
305.274518669	0.05	H-19->LUMO (44%), H-12->L+1 (25%)	H-20->LUMO (3%), H-18->LUMO (5%), H-17->LUMO (5%), H-11->L+1 (5%)
300.312929665	0.0022	H-20->LUMO (73%), H-19->LUMO (10%)	H-14->L+1 (5%)
295.277794213	0.068	H-14->L+1 (65%)	H-21->LUMO (6%), H-20->LUMO (5%), H-17->L+1 (3%), H-15->L+1 (5%), H-13->L+1 (6%)
292.215685056	0.007	H-16->L+1 (28%), H-15->L+1 (28%)	H-21->LUMO (6%), H-18->L+1 (5%), H-17->L+1 (8%), H-14->L+1 (6%), H-13->L+1 (7%)
290.429123945	0.0056	H-17->L+1 (15%), H-16->L+1 (40%)	H-22->LUMO (4%), H-19->L+1 (3%), H-18->L+1 (4%), H-15->L+1 (6%), H-14->L+1 (3%), H-13->L+1 (2%), H-4->L+2 (6%), H-4->L+3 (3%)
289.892662939	0.0276	H-21->LUMO (47%), H-18->L+1 (12%)	H-14->L+1 (3%), H-3->L+4 (4%), H-2->L+2 (2%), H-2->L+4 (8%), H-2->L+5 (3%)
288.798753843	0.0168	H-4->L+2 (21%), H-4->L+3 (21%), H-2->L+3 (15%), H-2->L+4 (12%)	H-21->LUMO (3%), H-16->L+1 (6%), H-14->L+1 (2%), H-3->L+4 (4%), H-2->L+5 (3%)
288.563499074	0.0665	H-4->L+3 (14%), H-2->L+2 (12%), H-2->L+4 (24%)	H-21->LUMO (8%), H-18->L+1 (7%), H-4->L+2 (4%), H-3->L+4 (8%), H-3->L+5 (3%), H-2->L+5 (5%)
286.914106894	0.0421	H-21->LUMO (11%), H-18->L+1 (21%), H-17->L+1 (37%)	H-20->LUMO (3%), H-16->L+1 (6%), H-13->L+1 (3%), HOMO->L+6 (3%)

Table S8. Selected TD-DFT calculated oscillator strengths and compositions of the major electronic transitions of **12**.

Wavelength (nm)	Osc. Strength	Major contributions	Minor contributions
582.085413203	0.0694	HOMO->LUMO (92%)	H-1->L+1 (3%)
523.140054904	0.0657	H-1->LUMO (53%), HOMO->L+1 (38%)	H-2->LUMO (5%)
501.128462925	0.0274	H-2->LUMO (84%)	H-4->LUMO (2%), H-3->LUMO (4%), HOMO->L+1 (2%)
486.7087737	0.1894	H-3->LUMO (17%), H-1->LUMO (31%), HOMO->L+1 (39%)	H-5->LUMO (5%), H-4->L+1 (3%), H-3->L+1 (3%)
479.666484882	0.0402	H-3->LUMO (66%), HOMO->L+1 (11%)	H-4->LUMO (5%), H-2->LUMO (2%), H-1->L+1 (9%)
468.962073577	0.0255	H-4->LUMO (62%), H-3->LUMO (10%), H-1->L+1 (18%)	H-5->LUMO (4%), H-1->LUMO (3%)
453.888537898	0.0251	H-5->LUMO (79%)	H-4->LUMO (8%), H-1->L+1 (3%), HOMO->L+1 (4%)
429.724778221	0.0512	H-2->L+1 (80%), H-1->L+1 (10%)	H-2->LUMO (2%)
411.96236381	0.298	H-5->L+1 (18%), H-3->L+1 (13%), H-2->L+1 (13%), H-1->L+1 (28%)	H-6->LUMO (3%), H-5->LUMO (6%), H-4->LUMO (5%), H-4->L+1 (9%)
404.146922916	0.2152	H-6->LUMO (10%), H-3->L+1 (69%)	H-5->L+1 (6%), H-1->L+1 (6%)
397.257907761	0.0652	H-8->LUMO (18%), H-7->LUMO (11%), H-6->LUMO (42%), H-4->L+1 (11%)	H-5->L+1 (5%), H-3->L+1 (4%)
393.900727577	0.3058	H-7->LUMO (42%), H-5->L+1 (38%)	H-6->LUMO (3%), H-4->LUMO (3%), H-1->L+1 (5%)
386.773749102	0.4065	H-7->LUMO (14%), H-6->LUMO (10%), H-4->L+1 (25%)	H-14->LUMO (6%), H-13->LUMO (9%), H-8->LUMO (5%), H-5->LUMO (2%), H-5->L+1 (4%), H-4->LUMO (3%), H-1->L+1 (8%)
385.103876416	0.3609	H-8->LUMO (16%), H-7->LUMO (13%), H-6->LUMO (15%), H-4->L+1 (28%)	H-15->LUMO (2%), H-14->LUMO (3%), H-13->LUMO (4%), H-10->LUMO (3%), H-5->L+1 (8%), H-1->LUMO (2%)
373.277714925	0.7088	H-8->LUMO (40%), H-6->LUMO (14%), H-5->L+1 (10%), H-4->L+1 (12%)	H-7->LUMO (5%), H-3->L+1 (4%), H-1->L+1 (2%)
370.124165658	0.0741	H-14->LUMO (18%), H-13->LUMO (24%), H-8->LUMO (12%), H-7->LUMO (12%)	H-15->LUMO (8%), H-10->LUMO (7%), H-5->L+1 (3%), H-4->LUMO (3%)
354.869176863	0.0075	H-9->LUMO (83%)	H-10->LUMO (6%), H-8->LUMO (2%), H-7->L+1 (2%)
352.047796616	0.0044	H-11->LUMO (70%), H-10-	H-9->LUMO (4%), H-8->L+1

		>LUMO (13%)	(4%), H-6->L+1 (2%)
351.838000545	0.0649	H-11->LUMO (16%), H-10->LUMO (64%)	H-14->LUMO (3%), H-13->LUMO (5%), H-9->LUMO (4%)
349.005469422	0.0096	H-8->L+1 (19%), H-7->L+1 (25%), H-6->L+1 (36%)	H-11->LUMO (5%), H-10->L+1 (2%)
346.256857632	0.0047	H-14->LUMO (16%), H-12->LUMO (76%)	
344.735695849	0.0217	H-7->L+1 (44%), H-6->L+1 (44%)	
342.412640538	0.0034	H-14->LUMO (39%), H-13->LUMO (43%), H-12->LUMO (13%)	
335.845797362	0.0032	H-15->LUMO (78%)	H-14->LUMO (5%), H-13->LUMO (5%), H-8->L+1 (3%)
335.400619521	0.056	H-13->L+1 (11%), H-8->L+1 (39%), H-7->L+1 (14%), H-6->L+1 (12%)	H-15->L+1 (3%), H-14->L+1 (6%), H-10->L+1 (2%)
331.739158271	0.0195	H-20->LUMO (13%), H-16->LUMO (24%), H-14->L+1 (10%), H-13->L+1 (10%), H-8->L+1 (14%)	H-19->LUMO (5%), H-18->LUMO (2%), H-15->L+1 (4%)
329.841690421	0.023	H-16->LUMO (52%), H-14->L+1 (10%), H-13->L+1 (13%)	H-15->L+1 (4%), H-8->L+1 (9%)
328.104670827	0.0049	H-17->LUMO (92%)	
325.528902282	0.0021	H-20->LUMO (24%), H-18->LUMO (25%), H-16->LUMO (18%)	H-21->LUMO (6%), H-19->LUMO (9%), H-13->L+1 (3%), H-8->L+1 (3%)
321.052858802	0.0086	H-20->LUMO (23%), H-18->LUMO (60%)	H-21->LUMO (6%), H-19->LUMO (3%)
318.275428089	0.0047	H-19->LUMO (49%), H-11->L+1 (11%), H-9->L+1 (16%)	H-21->LUMO (3%), H-20->LUMO (9%), H-10->L+1 (4%)
316.601192544	0.014	H-19->LUMO (22%), H-9->L+1 (57%)	H-20->LUMO (6%)
315.810879065	0.0393	H-11->L+1 (23%), H-10->L+1 (49%)	H-20->LUMO (3%), H-19->LUMO (3%), H-14->L+1 (3%), H-9->L+1 (8%), H-7->L+1 (2%)
313.923770128	0.0109	H-11->L+1 (50%), H-10->L+1 (35%)	H-21->LUMO (2%), H-13->L+1 (3%)
309.596706401	0.0028	H-12->L+1 (69%)	H-22->LUMO (5%), H-21->LUMO (8%), H-15->L+1 (3%), H-11->L+1 (4%)
305.929856669	0.0083	H-22->LUMO (16%), H-14->L+1 (45%), H-13->L+1 (13%)	H-21->LUMO (5%), H-15->L+1 (3%), H-12->L+1 (3%), H-9->L+1 (4%), HOMO->L+2 (7%)

305.628202756	0.0201	H-22->LUMO (24%), H-14->L+1 (13%), H-13->L+1 (12%), HOMO->L+2 (28%)	H-21->LUMO (3%), H-18->LUMO (2%), H-15->L+1 (2%), H-12->L+1 (7%), H-9->L+1 (2%)
303.853036497	0.0943	H-22->LUMO (12%), H-21->LUMO (15%), HOMO->L+2 (51%)	H-13->L+1 (4%), H-12->L+1 (6%), H-9->L+1 (2%)
301.76749504	0.0105	H-15->L+1 (68%), H-13->L+1 (19%)	
301.628008788	0.1132	H-22->LUMO (29%), H-21->LUMO (31%), H-1->L+2 (11%)	H-20->LUMO (8%), H-20->L+1 (2%), H-12->L+1 (3%), HOMO->L+2 (6%)
294.737300937	0.0106	H-16->L+1 (88%)	H-1->L+2 (6%)
294.485281013	0.0091	H-18->L+1 (18%), H-17->L+1 (60%)	H-20->L+1 (2%), H-15->L+1 (4%), H-1->L+2 (9%)
291.30255395	0.015	H-18->L+1 (61%), H-17->L+1 (25%)	H-22->L+1 (2%), H-20->L+1 (3%)
290.776502761	0.1656	H-1->L+2 (57%)	H-22->LUMO (2%), H-21->LUMO (8%), H-20->LUMO (3%), H-20->L+1 (2%), H-19->L+1 (4%), H-18->L+1 (4%), H-17->L+1 (5%), H-16->L+1 (3%), H-2->L+2 (3%)
286.238469381	0.009	H-20->L+1 (25%), H-19->L+1 (51%)	H-21->L+1 (5%), H-1->L+2 (7%)
282.334091661	0.0053	H-20->L+1 (42%), H-19->L+1 (39%)	H-22->L+1 (3%), H-21->L+1 (4%), H-18->L+1 (3%)
280.837621211	0.0683	H-2->L+2 (84%)	H-22->L+1 (2%), H-1->L+2 (3%)
277.997697285	0.0322	H-3->L+2 (59%), HOMO->L+4 (13%)	H-21->L+1 (6%), H-20->L+1 (2%), H-4->L+2 (2%), H-2->L+2 (2%), HOMO->L+3 (7%)
277.26411211	0.0132	H-3->L+2 (19%), HOMO->L+4 (68%)	H-18->L+1 (2%)
276.324841232	0.0143	H-21->L+1 (11%), HOMO->L+3 (57%)	H-22->L+1 (2%), H-3->L+2 (8%), HOMO->L+4 (5%), HOMO->L+5 (4%)

Table S9. Selected TD-DFT calculated oscillator strengths and compositions of the major electronic transitions of **13**.

Wavelength (nm)	**Osc. Strength**	**Major contributions**	**Minor contributions**
564.976956082	0.0951	HOMO->LUMO (84%)	H-2->LUMO (2%), H-1->LUMO (4%), H-1->L+1 (6%)
521.358197772	0.1008	H-1->LUMO (61%), HOMO->L+1 (31%)	HOMO->LUMO (5%)

485.546085813	0.076	H-2->LUMO (68%), HOMO->L+1 (12%)	H-3->L+1 (2%), H-1->LUMO (8%), H-1->L+1 (3%)
465.022102664	0.1928	H-3->LUMO (28%), H-2->LUMO (11%), H-1->LUMO (17%), HOMO->L+1 (34%)	H-3->L+1 (7%)
462.38604092	0.0398	H-3->LUMO (55%), H-1->L+1 (20%), HOMO->L+1 (10%)	H-4->LUMO (3%), H-3->L+1 (3%), H-2->LUMO (5%)
435.689612441	0.0285	H-4->LUMO (79%)	H-3->LUMO (6%), H-2->LUMO (3%), H-1->L+1 (6%)
425.185847093	0.1163	H-5->LUMO (72%), H-1->L+1 (12%)	H-4->LUMO (5%), HOMO->LUMO (2%)
412.318566718	0.074	H-2->L+1 (87%)	H-3->L+1 (3%), H-2->LUMO (3%)
404.423762965	0.6346	H-5->LUMO (17%), H-1->L+1 (37%)	H-7->LUMO (5%), H-6->LUMO (9%), H-5->L+1 (3%), H-4->LUMO (5%), H-3->LUMO (4%), H-2->LUMO (3%), H-2->L+1 (5%), HOMO->LUMO (5%)
399.704029828	0.0048	H-7->LUMO (69%), H-6->LUMO (16%)	H-8->LUMO (3%), H-5->LUMO (3%)
392.939476475	0.0871	H-7->LUMO (15%), H-6->LUMO (57%)	H-11->LUMO (3%), H-5->L+1 (4%), H-4->L+1 (3%), H-3->L+1 (6%), H-1->L+1 (3%)
385.151728782	0.4508	H-11->LUMO (15%), H-8->LUMO (10%), H-3->L+1 (47%)	H-16->LUMO (3%), H-9->LUMO (4%), H-1->LUMO (3%), HOMO->L+1 (4%)
383.638198565	0.3654	H-11->LUMO (18%), H-8->LUMO (41%), H-3->L+1 (19%)	H-6->LUMO (8%)
380.447982486	0.0076	H-11->LUMO (32%), H-8->LUMO (38%)	H-16->LUMO (3%), H-9->LUMO (3%), H-7->LUMO (3%), H-5->L+1 (6%)
375.641377362	0.2659	H-5->L+1 (13%), H-4->L+1 (64%)	H-6->LUMO (4%)
371.176819484	0.2024	H-9->LUMO (40%), H-5->L+1 (27%), H-4->L+1 (14%)	H-16->LUMO (3%), H-10->LUMO (6%), H-1->L+1 (2%)
369.000574441	0.0031	H-9->LUMO (43%), H-5->L+1 (34%)	H-11->LUMO (7%), H-8->LUMO (2%), H-4->L+1 (9%)
365.099658448	0.0212	H-10->LUMO (81%)	H-12->LUMO (3%), H-5->L+1 (5%)
355.174152092	0.0182	H-13->LUMO (17%), H-12->LUMO (56%)	H-19->LUMO (3%), H-11->LUMO (4%), H-10->LUMO (4%), H-7->LUMO (2%), H-7->L+1 (2%)
348.838537539	0.0078	H-13->LUMO (27%), H-12->LUMO (17%), H-7->L+1	

		(22%), H-6->L+1 (23%)	
347.479591413	0.0259	H-13->LUMO (38%), H-7->L+1 (45%)	H-12->LUMO (5%), H-6->L+1 (3%)
344.534521792	0.0291	H-7->L+1 (15%), H-6->L+1 (66%)	H-13->LUMO (4%), H-12->LUMO (3%), H-11->L+1 (3%)
340.924995222	0.0212	H-16->LUMO (27%), H-11->L+1 (20%), H-8->L+1 (27%)	H-19->LUMO (2%), H-11->LUMO (4%), H-9->L+1 (5%)
338.514151183	0.0525	H-16->LUMO (26%), H-11->L+1 (30%), H-9->L+1 (11%)	H-18->LUMO (3%), H-15->LUMO (4%), H-13->L+1 (2%), H-11->LUMO (2%), H-7->L+1 (5%)
337.528089217	0.0036	H-14->LUMO (86%)	H-11->L+1 (2%), H-8->L+1 (2%), H-7->L+1 (2%)
334.829979238	0.0177	H-18->LUMO (15%), H-8->L+1 (44%)	H-20->LUMO (3%), H-16->LUMO (9%), H-15->LUMO (4%), H-14->LUMO (7%), H-11->L+1 (6%)
334.22523456	0.0323	H-15->LUMO (68%), H-8->L+1 (11%)	H-18->LUMO (5%), H-17->LUMO (4%), H-11->LUMO (2%)
331.952323995	0.0187	H-18->LUMO (18%), H-17->LUMO (22%), H-9->L+1 (37%)	H-20->LUMO (3%), H-15->LUMO (3%), H-11->L+1 (6%)
330.77446579	0.022	H-18->LUMO (22%), H-15->LUMO (10%), H-9->L+1 (30%)	H-19->LUMO (3%), H-17->LUMO (7%), H-16->LUMO (5%), H-16->L+1 (2%), H-11->L+1 (3%), H-10->L+1 (4%), H-8->L+1 (7%)
327.541259642	0.0034	H-20->LUMO (18%), H-19->LUMO (56%)	H-17->LUMO (6%), H-15->LUMO (2%), H-12->LUMO (4%)
326.360076368	0.0501	H-18->LUMO (20%), H-17->LUMO (53%)	H-19->LUMO (3%), H-16->LUMO (7%), H-10->L+1 (3%), H-9->L+1 (4%)
322.413712163	0.0047	H-10->L+1 (74%)	H-20->LUMO (4%), H-19->LUMO (3%), H-18->LUMO (4%), H-17->LUMO (2%)
321.510756456	0.0436	H-20->LUMO (55%), H-19->LUMO (15%)	H-21->LUMO (3%), H-18->LUMO (5%), H-13->L+1 (4%), H-11->LUMO (2%), H-10->L+1 (4%), H-9->L+1 (2%)
315.353019158	0.0285	H-13->L+1 (33%), H-12->L+1 (39%)	H-20->LUMO (3%), H-19->L+1 (2%), H-11->L+1 (7%), H-10->L+1 (5%)
311.572872144	0.0238	H-13->L+1 (48%), H-12->L+1 (39%)	H-16->L+1 (3%)
304.951651652	0.0005	H-16->L+1 (59%)	H-15->L+1 (4%), H-14->L+1

			(8%), H-12->L+1 (4%), H-11->L+1 (7%), H-10->L+1 (2%), HOMO->L+2 (9%)
300.830283429	0.0686	H-14->L+1 (47%), HOMO->L+2 (33%)	H-15->L+1 (9%), H-1->L+2 (2%)
299.536608553	0.0516	H-16->L+1 (13%), H-14->L+1 (37%), HOMO->L+2 (30%)	H-19->L+1 (6%), H-18->L+1 (3%)
297.666841958	0.0251	H-15->L+1 (59%), HOMO->L+2 (18%)	H-21->LUMO (7%), H-19->L+1 (5%), H-12->L+1 (2%)
296.797512836	0.0286	H-21->LUMO (27%), H-17->L+1 (22%), H-15->L+1 (12%)	H-19->L+1 (8%), H-18->L+1 (8%), H-16->L+1 (5%), H-14->L+1 (3%), H-1->L+2 (9%)
295.545262359	0.0098	H-19->L+1 (14%), H-17->L+1 (58%), H-1->L+2 (12%)	H-22->LUMO (4%), H-15->L+1 (5%)
292.802269536	0.0358	H-20->L+1 (10%), H-19->L+1 (35%), H-1->L+2 (31%)	H-21->LUMO (4%), H-16->L+1 (3%), H-15->L+1 (2%), H-12->L+1 (2%), HOMO->L+2 (4%)
291.59715189	0.0113	H-18->L+1 (78%)	H-21->LUMO (4%), H-20->L+1 (3%), H-19->L+1 (5%)
289.007442919	0.1233	H-22->LUMO (11%), H-21->LUMO (44%), H-17->L+1 (12%), H-1->L+2 (18%)	H-20->LUMO (4%), H-19->L+1 (5%)
288.59708343	0.0704	H-22->LUMO (62%), H-1->L+2 (16%)	H-20->L+1 (7%), H-19->LUMO (3%)
283.043085134	0.0143	H-22->LUMO (12%), H-20->L+1 (69%)	H-19->L+1 (8%), H-18->L+1 (2%), H-1->L+2 (2%)
277.375764586	0.022	HOMO->L+3 (92%)	H-21->L+1 (2%)
272.768497849	0.1381	H-2->L+2 (71%), HOMO->L+4 (17%)	H-1->L+3 (3%)
271.537873439	0.0312	H-2->L+2 (20%), HOMO->L+4 (68%)	H-3->L+2 (2%)
269.255745243	0.0099	H-23->LUMO (47%), H-21->L+1 (13%), H-1->L+3 (28%)	

Table S10. Selected TD-DFT calculated oscillator strengths and compositions of the major electronic transitions of **14**

Wavelength (nm)	**Osc. Strength**	**Major contributions**	**Minor contributions**
559.293544804	0.0961	HOMO->LUMO (86%)	H-1->LUMO (3%), H-1->L+1 (7%)
514.73489024	0.1251	H-1->LUMO (60%), HOMO->L+1 (32%)	HOMO->LUMO (4%)
479.945004499	0.0599	H-2->LUMO (73%)	H-1->LUMO (7%), H-1->L+1 (3%), HOMO->L+1 (9%)
465.091878656	0.1189	H-3->LUMO (55%), H-1->LUMO (12%), HOMO-	H-4->LUMO (7%), H-3->L+1 (2%), H-2->LUMO (5%), H-1-

		>L+1 (13%)	>L+1 (3%)
462.903946432	0.1459	H-3->LUMO (13%), H-1->L+1 (16%), HOMO->L+1 (35%)	H-5->LUMO (2%), H-4->LUMO (8%), H-4->L+1 (2%), H-3->L+1 (4%), H-2->LUMO (9%), H-1->LUMO (8%)
448.69786122	0.0114	H-4->LUMO (66%), H-3->LUMO (23%)	H-2->LUMO (2%), H-1->L+1 (3%)
430.889667798	0.0665	H-5->LUMO (83%)	H-1->L+1 (7%)
409.256289857	0.0895	H-2->L+1 (87%)	H-2->LUMO (2%), H-1->L+1 (3%)
404.06789536	0.8342	H-6->LUMO (19%), H-1->L+1 (41%)	H-5->LUMO (7%), H-5->L+1 (2%), H-4->LUMO (8%), H-2->LUMO (3%), H-2->L+1 (5%), HOMO->LUMO (4%)
394.791253024	0.1873	H-8->LUMO (11%), H-6->LUMO (53%)	H-7->LUMO (5%), H-5->LUMO (4%), H-4->L+1 (5%), H-3->L+1 (3%), H-1->L+1 (7%)
392.665694417	0.1655	H-7->LUMO (21%), H-3->L+1 (57%)	H-8->LUMO (6%), H-5->L+1 (2%)
386.400077951	0.0786	H-14->LUMO (18%), H-8->LUMO (11%), H-7->LUMO (44%), H-3->L+1 (10%)	H-15->LUMO (5%)
383.317956445	0.4037	H-4->L+1 (65%)	H-8->LUMO (5%), H-6->LUMO (8%), H-5->L+1 (6%), H-1->L+1 (3%)
380.611490444	0.1962	H-8->LUMO (18%), H-6->LUMO (12%), H-5->L+1 (32%), H-3->L+1 (14%)	H-15->LUMO (2%), H-14->LUMO (6%), H-7->LUMO (4%)
373.96450809	0.4173	H-14->LUMO (11%), H-8->LUMO (31%), H-5->L+1 (25%), H-4->L+1 (13%)	H-15->LUMO (2%), H-6->LUMO (3%), H-3->L+1 (2%)
369.517458982	0.2353	H-14->LUMO (18%), H-7->LUMO (20%), H-5->L+1 (22%)	H-15->LUMO (8%), H-9->LUMO (9%), H-8->LUMO (5%), H-4->LUMO (4%), H-4->L+1 (2%)
359.676809527	0.0315	H-10->LUMO (12%), H-9->LUMO (70%)	H-14->LUMO (5%), H-12->LUMO (3%)
357.973705824	0.0092	H-11->LUMO (14%), H-10->LUMO (67%)	H-9->LUMO (8%)
354.747333368	0.0053	H-11->LUMO (72%), H-10->LUMO (14%)	H-14->LUMO (3%), H-9->LUMO (3%)
350.961567674	0.0027	H-13->LUMO (10%), H-12->LUMO (79%)	H-15->LUMO (4%)
348.946534047	0.0017	H-8->L+1 (19%), H-6->L+1 (52%)	H-14->L+1 (3%), H-13->LUMO (7%), H-7->L+1 (6%)
348.172403853	0.0014	H-13->LUMO (70%), H-12->LUMO (11%)	H-14->LUMO (5%), H-6->L+1 (7%)
343.180339383	0.0291	H-8->L+1 (14%), H-7->L+1 (42%), H-6->L+1	H-14->LUMO (2%), H-14->L+1 (3%), H-9->L+1 (2%)

		(27%)	
341.009387239	0.035	H-15->LUMO (67%), H-14->LUMO (18%)	H-13->LUMO (4%)
336.721417159	0.045	H-8->L+1 (35%), H-7->L+1 (37%)	H-19->LUMO (4%), H-14->L+1 (4%), H-6->L+1 (6%)
334.775733798	0.0185	H-19->LUMO (64%)	H-25->LUMO (8%), H-24->LUMO (5%), H-18->LUMO (6%), H-8->L+1 (4%)
332.575625033	0.0033	H-21->LUMO (33%), H-14->L+1 (23%)	H-25->LUMO (3%), H-19->LUMO (8%), H-15->L+1 (7%), H-13->L+1 (3%), H-8->L+1 (9%)
331.322500768	0.0147	H-21->LUMO (59%), H-14->L+1 (11%)	H-25->LUMO (3%), H-19->LUMO (6%), H-15->L+1 (3%), H-7->L+1 (2%)
328.269726528	0.0056	H-25->LUMO (28%), H-24->LUMO (20%), H-22->LUMO (13%)	H-23->LUMO (5%), H-19->LUMO (7%), H-15->L+1 (3%), H-14->L+1 (6%), H-8->L+1 (5%)
325.503263356	0.0003	H-25->LUMO (11%), H-22->LUMO (74%)	H-24->LUMO (3%), H-9->L+1 (3%)
322.774635562	0.0226	H-23->LUMO (16%), H-9->L+1 (59%)	H-22->LUMO (4%), H-11->L+1 (3%), H-10->L+1 (8%)
320.571395729	0.0345	H-23->LUMO (36%), H-10->L+1 (15%), H-9->L+1 (26%)	H-25->LUMO (7%), H-16->LUMO (4%), H-14->L+1 (3%)
319.893165314	0.0053	H-16->LUMO (47%), H-10->L+1 (36%)	H-23->LUMO (5%)
319.695201414	0.0066	H-23->LUMO (19%), H-16->LUMO (46%), H-10->L+1 (22%)	H-25->LUMO (3%)
318.242750102	0.0011	H-18->LUMO (27%), H-17->LUMO (67%)	
318.161084483	0.0001	H-18->LUMO (63%), H-17->LUMO (29%)	H-19->LUMO (6%)
317.558059094	0.001	H-20->LUMO (72%)	H-26->LUMO (7%), H-24->LUMO (3%), H-11->L+1 (7%)
316.860111458	0.0075	H-26->LUMO (13%), H-24->LUMO (10%), H-20->LUMO (23%), H-11->L+1 (32%)	H-25->LUMO (5%), H-12->L+1 (4%)
315.328958041	0.0049	H-26->LUMO (30%), H-11->L+1 (42%)	H-31->LUMO (3%), H-24->LUMO (2%), H-14->L+1 (4%), H-13->L+1 (2%), H-12->L+1 (2%)
313.30501355	0.0225	H-26->LUMO (18%), H-12->L+1 (57%)	H-13->L+1 (7%)
309.666299546	0.0303	H-14->L+1 (12%), H-13->L+1 (59%)	H-25->LUMO (3%), H-24->LUMO (7%), H-15->L+1 (6%), H-10->L+1 (3%)
308.840934144	0.1582	H-24->LUMO (21%), H-	H-26->LUMO (8%), H-25-

		13->L+1 (11%), H-12->L+1 (19%), HOMO->L+2 (10%)	>LUMO (6%), H-10->L+1 (3%), H-1->L+2 (8%), HOMO->L+3 (3%)
307.912861998	0.2826	HOMO->L+2 (73%)	H-15->L+1 (6%), H-12->L+1 (5%)
306.338035264	0.0803	H-15->L+1 (58%), H-14->L+1 (11%)	H-25->LUMO (3%), H-24->LUMO (6%), H-13->L+1 (7%), HOMO->L+2 (5%)
300.662494877	0.0813	HOMO->L+3 (82%)	H-22->L+1 (3%), H-21->L+1 (3%)
298.390394966	0.013	H-19->L+1 (76%), H-1->L+2 (10%)	H-18->L+1 (6%)
297.781230215	0.0156	H-21->L+1 (48%), H-1->L+2 (26%)	H-22->L+1 (9%)
296.627094627	0.191	H-1->L+2 (12%), HOMO->L+4 (75%)	
295.770874811	0.058	H-21->L+1 (23%), H-1->L+2 (28%), HOMO->L+4 (15%)	H-24->LUMO (4%), H-23->L+1 (3%), H-22->L+1 (4%), H-19->L+1 (5%), HOMO->L+3 (3%)
293.217749059	0.0125	H-22->L+1 (66%), H-21->L+1 (17%)	HOMO->L+5 (5%)

Table S11. S_0 optimized geometry of compound **8** at B3LYP/6-31g (d,p) level of theory.

Sum of imaginary frequencies= 0

Total Energy (hartree) = -12146.44981290

Atom	X	Y	Z	Atom	X	Y	Z
Br	4.01548	-2.5388	-1.2258	C	5.20502	4.65151	-0.5831
Br	1.11154	-4.3969	-1.2584	H	5.64066	5.19044	-1.4209
Br	-5.441	1.32679	0.85774	C	5.63579	4.93598	0.71836
Br	-4.6186	-2.0478	1.27417	C	-3.5344	-0.7937	0.38817
N	0.07313	1.99632	-0.2464	C	-2.3209	2.54055	-0.5176
H	-0.0203	0.96686	-0.0801	C	-3.3337	3.61224	-0.6207
N	0.67428	-0.5311	0.09132	C	-2.7089	-3.9583	-0.7743
N	-1.7614	0.22897	-0.6125	H	-3.0928	-3.3458	-1.5842
C	1.99489	-0.5483	-0.1401	C	-3.8568	0.53222	0.23181
C	3.64575	2.97253	0.23088	C	-3.2799	4.76798	0.17634
C	2.54811	1.9638	-0.0098	H	-2.5001	4.8631	0.92496
C	-0.9465	2.88034	-0.5254	C	-1.2498	-4.2383	1.12631
C	4.29623	0.23439	0.35441	H	-0.5031	-3.84	1.80607
C	1.27958	2.60235	-0.2632	C	-1.7215	-5.5357	1.29237

C	2.87193	0.59851	0.04561	H	-1.3364	-6.1441	2.10653
C	0.13608	-1.7663	-0.1723	C	-2.6782	-6.0751	0.42143
C	5.3657	0.55306	-0.4936	C	8.36323	-0.9228	1.35563
H	5.17539	1.08255	-1.4204	H	8.85829	-0.1286	1.92879
C	-0.3159	4.15361	-0.7396	H	8.96656	-1.0994	0.46006
H	-0.8316	5.06436	-1.0044	H	8.39067	-1.8295	1.96715
C	4.06623	3.26297	1.53511	C	-4.2341	5.77274	0.03819
H	3.62251	2.72862	2.36967	H	-4.178	6.65208	0.6747
C	2.36576	-1.892	-0.5944	C	-3.1558	-5.2654	-0.6188
C	1.2182	-2.6409	-0.5962	H	-3.891	-5.6649	-1.3126
C	-2.1779	-0.9553	-0.1313	C	-4.3785	3.49982	-1.5552
C	-1.2533	-2.0415	-0.08	H	-4.434	2.61712	-2.1845
C	4.22652	3.68738	-0.8247	C	6.71844	5.95659	0.97732
H	3.90985	3.48622	-1.8445	H	6.55972	6.477	1.92679
C	5.87742	-0.8576	1.84453	H	6.76009	6.707	0.18246
H	6.06452	-1.4135	2.75992	H	7.70633	5.48202	1.02953
C	-2.6924	1.17074	-0.3731	C	-5.2679	5.66724	-0.901
C	1.03668	3.99216	-0.5608	C	-3.2005	-7.4779	0.6147
H	1.79687	4.75274	-0.6418	H	-2.4558	-8.1203	1.09356
C	-1.7394	-3.4262	0.09096	H	-3.4829	-7.9348	-0.3383
C	6.94713	-0.5381	1.00047	H	-4.0927	-7.4814	1.25354
C	4.57342	-0.4859	1.52474	C	-5.3181	4.51395	-1.6975
H	3.75798	-0.7577	2.18892	H	-6.1064	4.41027	-2.4386
C	6.66445	0.17	-0.1758	C	-6.3148	6.74642	-1.0319
H	7.47424	0.41658	-0.8581	H	-7.1936	6.51887	-0.4156
C	5.04506	4.22587	1.77164	H	-6.6614	6.84437	-2.065
H	5.35231	4.43243	2.79396	H	-5.9322	7.7182	-0.7071

Table S12. S_0 optimized geometry of compound 9 at B3LYP/6-31g (d,p) level of theory.

Sum of imaginary frequencies= 0

Total Energy (hartree) = -2786.27905167

Atom	X	Y	Z	Atom	X	Y	Z
C	2.848672	-1.05496	0.27881	C	6.256174	2.621589	-0.86167

C	2.427159	-2.37379	0.086464	C	6.565997	2.111546	-2.12296
C	2.096194	0.173032	0.033529	C	5.606353	1.379592	-2.82374
C	4.221173	-0.81237	0.84136	C	4.347435	1.160707	-2.26518
C	3.395974	-3.49749	0.361797	C	1.643651	3.649839	-1.20296
C	1.138373	-2.86136	-0.35135	C	2.472046	4.677734	-0.72745
C	2.65888	1.443233	-0.45008	C	2.544574	5.903298	-1.38885
C	1.597221	2.32322	-0.54259	C	1.790261	6.125858	-2.54097
C	0.407125	1.573373	-0.12065	C	0.962462	5.111737	-3.02615
N	0.779067	0.292815	0.213237	C	0.891226	3.887041	-2.36547
N	-0.01012	-2.14845	-0.34663	H	-0.0245	-1.13616	-0.07725
C	-1.07461	-2.89514	-0.80418	H	-1.10593	-5.00886	-1.53471
C	-0.53982	-4.18658	-1.12357	H	1.503603	-4.98817	-0.95159
C	0.805968	-4.17416	-0.83158	H	0.192578	3.824401	1.564857
C	-0.94968	1.988662	-0.07717	H	-0.4345	6.194221	1.844322
C	-2.41423	-2.4246	-0.84777	H	-3.54135	5.715241	-1.07971
C	-1.97033	0.980299	-0.1832	H	-2.91269	3.347584	-1.35935
C	-3.35173	0.912815	0.33117	H	-2.84416	-4.87463	0.312969
C	-3.8009	-0.364	0.036127	H	-4.637	-6.48151	-0.20987
C	-2.66923	-1.04189	-0.61435	H	-6.25276	-3.74367	-3.09463
N	-1.6429	-0.17996	-0.76715	H	-4.45428	-2.13633	-2.57408
C	-1.31131	3.408839	0.080712	H	3.408018	0.141181	2.591347
C	-3.50304	-3.3905	-1.10593	H	5.599903	0.566561	3.643499
C	-0.62038	4.240189	0.978779	H	7.55417	-1.22204	0.266214
C	-0.9807	5.57367	1.138502	H	5.371874	-1.66378	-0.76951
C	-2.03844	6.130717	0.408144	H	3.120406	-3.43713	2.495949
C	-2.72335	5.303919	-0.49379	H	4.653325	-5.31123	2.959335
C	-2.37432	3.968366	-0.6506	H	5.42617	-5.71891	-1.24294
C	-3.57559	-4.63255	-0.45103	H	3.896204	-3.83891	-1.7046
C	-4.59408	-5.53523	-0.74337	H	8.018498	0.657653	3.502162
C	-5.57165	-5.24129	-1.70306	H	8.814818	0.320837	1.956918
C	-5.50353	-3.9996	-2.34975	H	8.5074	-0.98975	3.094644
C	-4.49522	-3.08848	-2.05494	H	6.727182	-7.0382	0.328884
C	4.317186	-0.16673	2.082884	H	6.70885	-6.62667	2.050417

C	5.556798	0.073767	2.675098	H	5.506858	-7.73764	1.396253
C	6.744285	-0.30556	2.041006	H	-1.62141	8.1747	0.98433
C	6.646724	-0.93334	0.790927	H	-3.26992	7.646241	1.332552
C	5.412213	-1.18864	0.203491	H	-2.80244	8.017258	-0.32695
C	3.622104	-3.93737	1.6731	H	-7.5861	-5.73555	-2.32019
C	4.489862	-4.99556	1.931598	H	-6.35916	-6.8654	-2.8942
C	5.154545	-5.66123	0.892585	H	-6.86257	-6.90459	-1.20341
C	4.920969	-5.22516	-0.41633	H	-4.18962	-1.89718	2.223854
C	4.055622	-4.16219	-0.67948	H	-6.3102	-2.87633	3.045859
C	8.089667	-0.06277	2.682318	H	-8.42589	-2.49939	1.793346
C	6.07466	-6.8241	1.180069	H	-8.39475	-1.14322	-0.29115
C	-2.45019	7.568682	0.607043	H	-6.26798	-0.18177	-1.11436
C	-6.65351	-6.23678	-2.04415	H	-2.50891	1.966656	2.671495
C	-5.078	-0.96743	0.498384	H	-3.68506	3.583702	4.12503
C	-5.11053	-1.73799	1.670862	H	-5.9248	4.450922	3.473177
C	-6.30613	-2.28652	2.133506	H	-6.96712	3.681845	1.349277
C	-7.49378	-2.07474	1.431753	H	-5.77899	2.077655	-0.10604
C	-7.47571	-1.31302	0.262968	H	4.768317	2.785645	0.684449
C	-6.27844	-0.7664	-0.19897	H	6.997452	3.190498	-0.30739
C	-4.0573	1.904382	1.175591	H	7.546853	2.284222	-2.55679
C	4.022711	1.669132	-0.99708	H	5.835054	0.983143	-3.80918
C	-3.48267	2.347168	2.3791	H	3.598847	0.598678	-2.81601
C	-4.14788	3.257044	3.197999	H	3.05443	4.516119	0.173208
C	-5.40529	3.742823	2.833878	H	3.191616	6.685433	-1.00143
C	-5.98948	3.309985	1.643365	H	1.84731	7.079977	-3.05707
C	-5.32219	2.400774	0.823083	H	0.373975	5.272093	-3.9252
C	4.995781	2.404141	-0.30557	H	0.25494	3.097546	-2.75336

Table S13. S_0 optimized geometry of compound 10 at B3LYP/6-31g (d,p) level of theory.

Sum of imaginary frequencies= 0

Total Energy (hartree) = -3183.20813819

Atom	X	Y	Z	Atom	X	Y	Z
C	-2.8206	-1.448	0.40597	C	-5.9225	0.96502	-2.4541

C	-2.3203	-2.7321	0.1669	C	-6.8558	1.57605	-1.6263
C	-2.1673	-0.1665	0.15447	C	-6.5258	2.02544	-0.3541
C	-4.1811	-1.3162	1.0322	C	-5.2181	1.85501	0.09777
C	-3.199	-3.9229	0.46269	C	-2.0133	3.36483	-0.999
C	-1.0251	-3.1253	-0.3398	C	-1.3467	3.69367	-2.1917
C	-2.8368	1.07712	-0.2574	C	-1.53	4.93018	-2.806
C	-1.8399	2.02464	-0.3905	C	-2.3949	5.84591	-2.2189
C	-0.5814	1.34394	-0.0624	C	-3.0765	5.55988	-1.0434
N	-0.8509	0.03498	0.25533	C	-2.8799	4.31783	-0.4416
N	0.07058	-2.3354	-0.3863	F	-8.1226	1.73667	-2.0707
C	1.15823	-3.0039	-0.9059	F	-2.5772	7.04855	-2.809
C	0.69678	-4.3273	-1.2115	F	5.8689	4.78332	3.30407
C	-0.6292	-4.4094	-0.8511	F	8.84678	-2.1853	1.2806
C	0.74609	1.84892	-0.0852	H	0.02985	-1.3266	-0.1052
C	2.45778	-2.4428	-1.0159	H	1.29568	-5.1057	-1.6599
C	1.82472	0.91781	-0.2746	H	-1.2752	-5.2682	-0.944
C	3.23644	0.93974	0.15318	H	2.5108	3.38876	-1.4551
C	3.75199	-0.3004	-0.1862	H	2.98228	5.7878	-1.1402
C	2.63161	-1.0475	-0.7774	H	0.08164	5.9432	2.02111
N	1.54281	-0.2567	-0.8554	H	-0.3904	3.54287	1.70457
C	1.01622	3.28764	0.09374	H	4.3732	-2.0104	-2.8544
C	3.59424	-3.33	-1.3419	H	6.24906	-3.4861	-3.479
C	1.97808	3.94691	-0.6919	H	4.98866	-6.3354	-0.5255
C	2.23868	5.30047	-0.5148	H	3.11703	-4.8608	0.10017
C	1.56031	6.04861	0.45821	H	-5.3384	-2.1856	-0.5644
C	0.61066	5.38914	1.24992	H	-7.5015	-1.924	0.56914
C	0.33787	4.03749	1.07007	H	-5.5308	-0.1357	3.93707
C	4.50901	-2.9575	-2.3419	H	-3.3606	-0.3763	2.78633
C	5.56164	-3.7951	-2.6956	H	-3.7701	-4.2599	-1.5863
C	5.7528	-5.0295	-2.0597	H	-5.1492	-6.2459	-1.0962
C	4.85099	-5.3936	-1.0507	H	-4.2118	-5.8635	3.0749
C	3.78853	-4.5659	-0.6996	H	-2.8308	-3.8817	2.58332
C	-5.37	-1.7473	0.4262	H	-8.7988	-0.5727	2.35828

C	-6.594	-1.595	1.06944	H	-7.9643	-0.1701	3.86765
C	-6.6812	-1.0213	2.34603	H	-8.3294	-1.8526	3.47554
C	-5.4955	-0.5881	2.94887	H	-6.1787	-7.3194	2.25384
C	-4.2679	-0.7242	2.30076	H	-6.3121	-7.6564	0.52109
C	-3.8604	-4.6114	-0.562	H	-4.9703	-8.3235	1.45451
C	-4.6401	-5.7345	-0.2828	H	2.87006	7.7705	0.405
C	-4.7827	-6.2097	1.02582	H	1.61214	7.85403	1.6495
C	-4.1171	-5.5193	2.04778	H	1.19982	8.1177	-0.0461
C	-3.335	-4.3999	1.77317	H	7.22522	-6.5521	-1.618
C	-8.0116	-0.8932	3.04841	H	6.56668	-6.6385	-3.2524
C	-5.6068	-7.4388	1.32816	H	7.73766	-5.3828	-2.8456
C	1.82814	7.52347	0.62942	H	6.11739	0.08677	-1.4885
C	6.88225	-5.9461	-2.4617	H	8.37803	-0.7319	-0.815
C	5.09738	-0.8133	0.18093	H	6.6669	-2.6673	2.60049
C	6.23089	-0.5089	-0.5879	H	4.40482	-1.8381	1.94403
C	7.49784	-0.9646	-0.2254	H	5.53028	2.30096	-0.4362
C	7.62323	-1.7376	0.92156	H	6.70119	3.98494	0.98013
C	6.52685	-2.0643	1.7099	H	3.66739	3.58735	3.97645
C	5.26878	-1.5978	1.3324	H	2.49675	1.88938	2.57401
C	3.9261	1.97011	0.96341	H	-3.8764	0.33495	-2.6228
C	-4.2454	1.24096	-0.7041	H	-6.2173	0.6338	-3.444
C	5.1194	2.56986	0.53048	H	-7.2845	2.49457	0.26275
C	5.78085	3.51647	1.31171	H	-4.9544	2.18014	1.09843
C	5.2366	3.86402	2.54089	H	-0.6819	2.96602	-2.6457
C	4.05872	3.29354	3.00857	H	-1.0207	5.18808	-3.7281
C	3.41276	2.34806	2.21605	H	-3.7425	6.3007	-0.6145
C	-4.6197	0.8029	-1.9847	H	-3.3993	4.08854	0.4821

Table S14. S_0 optimized geometry of compound **11** at B3LYP/6-31g (d,p) level of theory.

Sum of imaginary frequencies= 0

Total Energy (hartree) = -3155.25238532

Atom	X	Y	Z	Atom	X	Y	Z
C	-2.777	-1.6737	0.49094	C	-6.6284	1.66407	-0.0585

C	-2.2356	-2.9354	0.22263	C	-5.3019	1.53566	0.33669
C	-2.1818	-0.365	0.23386	C	-2.205	3.17757	-0.8888
C	-4.1237	-1.6	1.15385	C	-1.5823	3.54234	-2.0958
C	-3.0584	-4.162	0.5322	C	-1.8332	4.772	-2.6904
C	-0.9427	-3.2731	-0.3286	C	-2.7258	5.67447	-2.088
C	-2.9124	0.85691	-0.1329	C	-3.3597	5.32099	-0.8863
C	-1.9573	1.84344	-0.2965	C	-3.0979	4.08802	-0.3001
C	-0.6632	1.20816	-0.0276	C	-8.3923	1.35883	-1.7453
N	-0.8715	-0.1107	0.28715	N	-9.505	1.45183	-2.0727
N	0.11888	-2.4418	-0.4073	C	-2.9827	6.94783	-2.6934
C	1.21309	-3.0654	-0.9698	N	-3.1866	7.98342	-3.1835
C	0.79164	-4.4048	-1.2686	C	5.7767	4.95993	3.20355
C	-0.5155	-4.5394	-0.8626	N	6.29674	5.77825	3.8471
C	0.64211	1.76735	-0.0948	C	9.00415	-2.0791	0.96008
C	2.48167	-2.4536	-1.1251	N	10.0745	-2.4579	1.21473
C	1.74625	0.88078	-0.3345	H	0.05124	-1.4386	-0.1171
C	3.16988	0.95531	0.03841	H	1.40322	-5.1563	-1.7448
C	3.71814	-0.2658	-0.3246	H	-1.132	-5.4211	-0.939
C	2.60673	-1.0513	-0.8774	H	2.28833	3.38558	-1.5182
N	1.49024	-0.3012	-0.9134	H	2.6797	5.79771	-1.1967
C	0.86358	3.21183	0.09068	H	-0.1045	5.8159	2.0712
C	3.64345	-3.2827	-1.504	H	-0.4988	3.40225	1.74897
C	1.77076	3.91454	-0.7242	H	4.29937	-1.9131	-3.0321
C	1.98582	5.27482	-0.5437	H	6.22423	-3.2855	-3.7353
C	1.3207	5.9878	0.46599	H	5.20609	-6.2279	-0.7794
C	0.42051	5.28732	1.27998	H	3.28435	-4.8583	-0.0743
C	0.19106	3.9276	1.09633	H	-5.2848	-2.5076	-0.4192
C	4.50439	-2.8533	-2.5299	H	-7.4285	-2.3329	0.76724
C	5.58483	-3.6328	-2.9279	H	-5.4448	-0.4956	4.10129
C	5.86294	-4.8598	-2.3085	H	-3.2964	-0.6424	2.89626
C	5.0087	-5.2845	-1.2818	H	-3.6766	-4.5026	-1.5035
C	3.91736	-4.5163	-0.8867	H	-4.9605	-6.5452	-0.9937
C	-5.3095	-2.0738	0.57372	H	-3.9155	-6.1649	3.15209

C	-6.5224	-1.9721	1.24725	H	-2.6301	-4.1248	2.64203
C	-6.6	-1.4109	2.53044	H	-7.8792	-0.6181	4.08652
C	-5.4167	-0.9374	3.10824	H	-8.1802	-2.3139	3.69814
C	-4.2014	-1.0204	2.42907	H	-8.7339	-1.0541	2.59744
C	-3.722	-4.8665	-0.4805	H	-5.7867	-7.7221	2.40384
C	-4.4478	-6.022	-0.1903	H	-6.0605	-7.9823	0.67409
C	-4.5319	-6.5151	1.11726	H	-4.6259	-8.6503	1.45527
C	-3.8649	-5.8078	2.1264	H	2.53322	7.6081	1.21689
C	-3.1364	-4.655	1.84105	H	0.79681	7.92854	1.26592
C	-7.9163	-1.3405	3.26641	H	1.67086	7.98938	-0.2732
C	-5.2945	-7.7809	1.42828	H	7.96186	-5.3478	-2.1789
C	1.58918	7.45651	0.67918	H	6.92057	-6.7394	-2.4844
C	7.063	-5.6796	-2.7133	H	7.26953	-5.5859	-3.7835
C	5.08891	-0.7373	-0.0054	H	6.03952	0.28333	-1.6474
C	6.1941	-0.35	-0.7797	H	8.32446	-0.4761	-1.0741
C	7.47865	-0.7804	-0.4668	H	6.74706	-2.659	2.28185
C	7.68444	-1.62	0.63938	H	4.46725	-1.8783	1.71285
C	6.58824	-2.0144	1.424	H	5.38952	2.41355	-0.6068
C	5.30997	-1.5752	1.10001	H	6.52752	4.11774	0.77344
C	3.84408	2.00193	0.83801	H	3.58702	3.56605	3.86604
C	-4.3422	0.97738	-0.5207	H	2.46628	1.84538	2.48821
C	4.99938	2.65384	0.37545	H	-4.0144	0.13556	-2.4765
C	5.63924	3.61839	1.14545	H	-6.3742	0.36084	-3.1988
C	5.13066	3.95709	2.40926	H	-7.3638	2.09041	0.61529
C	3.97816	3.31038	2.88713	H	-5.0081	1.84569	1.3333
C	3.35067	2.34654	2.10931	H	-0.9003	2.84596	-2.5721
C	-4.749	0.55858	-1.7985	H	-1.3478	5.04017	-3.6228
C	-6.0716	0.68399	-2.2084	H	-4.0483	6.01629	-0.4183
C	-7.0235	1.23721	-1.3367	H	-3.5813	3.83029	0.6352

Table S15. S_0 optimized geometry of compound **12** at B3LYP/6-31g (d,p) level of theory.

Sum of imaginary frequencies= 0

Total Energy (hartree) = -3244.37887087

Atom	X	Y	Z	Atom	X	Y	Z
C	-2.8014	-1.7438	0.5665	C	-3.4099	5.25714	-0.7872
C	-2.2674	-3.0047	0.27976	C	-3.1398	4.02248	-0.213
C	-2.2127	-0.4348	0.3014	O	-8.4328	1.36625	-1.4045
C	-4.1313	-1.6772	1.26491	O	-3.129	6.85718	-2.4802
C	-3.0866	-4.2316	0.59882	O	5.87647	4.82828	3.03017
C	-0.9882	-3.3439	-0.3003	O	8.90702	-2.1494	0.93367
C	-2.9511	0.7886	-0.0515	C	-8.921	0.98036	-2.6777
C	-1.9983	1.77228	-0.2358	C	-2.5469	7.26995	-3.7046
C	-0.6975	1.13441	0.00991	C	5.43526	5.21191	4.32124
N	-0.9	-0.1878	0.32438	C	10.0358	-1.7781	0.16144
N	0.07413	-2.5129	-0.3952	H	0.01003	-1.508	-0.1009
C	1.15573	-3.1341	-0.9804	H	1.33082	-5.221	-1.7666
C	0.7282	-4.4702	-1.2778	H	-1.1904	-5.488	-0.9171
C	-0.573	-4.6062	-0.8482	H	2.25787	3.29542	-1.506
C	0.60774	1.68844	-0.0755	H	2.66873	5.70494	-1.1907
C	2.42705	-2.5226	-1.1504	H	-0.1116	5.74975	2.08057
C	1.70981	0.79976	-0.3295	H	-0.5174	3.33699	1.76687
C	3.14161	0.8692	0.02687	H	4.22574	-1.9947	-3.0782
C	3.68461	-0.3455	-0.3588	H	6.11392	-3.3949	-3.8293
C	2.56184	-1.1263	-0.9018	H	5.11773	-6.3279	-0.8571
N	1.44075	-0.3763	-0.9121	H	3.23411	-4.9298	-0.1072
C	0.83755	3.13469	0.10599	H	-5.3359	-2.5448	-0.2964
C	3.57604	-3.3634	-1.5496	H	-7.4462	-2.4003	0.95387
C	1.74379	3.8305	-0.7141	H	-5.3686	-0.6449	4.2741
C	1.96979	5.18958	-0.5366	H	-3.2532	-0.7687	3.00691
C	1.31251	5.90817	0.47279	H	-3.7477	-4.5565	-1.4245
C	0.41143	5.21585	1.29124	H	-5.0229	-6.6035	-0.904
C	0.17552	3.85635	1.11303	H	-3.8921	-6.2539	3.22172
C	4.42129	-2.9445	-2.591	H	-2.6152	-4.2111	2.6988
C	5.48171	-3.7393	-3.0148	H	-8.4989	-0.6014	3.05789
C	5.74993	-4.9745	-2.4106	H	-7.7118	-1.1992	4.52292
C	4.91845	-5.3845	-1.3594	H	-8.4569	-2.3327	3.38514

C	3.84917	-4.6001	-0.9381	H	-5.8068	-7.7916	2.48779
C	-5.3335	-2.1348	0.70682	H	-6.0687	-8.0689	0.75899
C	-6.5268	-2.0486	1.41581	H	-4.6355	-8.7228	1.55532
C	-6.5689	-1.5134	2.71131	H	1.6771	7.90762	-0.2704
C	-5.3692	-1.0605	3.26919	H	2.53699	7.52534	1.21979
C	-4.1726	-1.1305	2.55524	H	0.80131	7.85517	1.26783
C	-3.7728	-4.9286	-0.4038	H	7.3564	-6.3799	-2.0544
C	-4.4934	-6.0861	-0.1075	H	6.53335	-6.6042	-3.5979
C	-4.5507	-6.5889	1.19742	H	7.65756	-5.2591	-3.3925
C	-3.8622	-5.8894	2.1976	H	5.9855	0.16514	-1.7398
C	-3.1388	-4.7354	1.90515	H	8.26799	-0.5637	-1.2135
C	-7.8748	-1.4082	3.46181	H	6.79593	-2.6857	2.22209
C	-5.3079	-7.8565	1.51571	H	4.48997	-1.9285	1.69052
C	1.59161	7.37627	0.68299	H	5.36788	2.31268	-0.6464
C	6.88622	-5.8468	-2.8865	H	6.53244	4.02206	0.72257
C	5.06196	-0.8181	-0.0665	H	3.6228	3.48453	3.83975
C	6.15222	-0.4536	-0.8627	H	2.48562	1.78747	2.48634
C	7.45295	-0.872	-0.5694	H	-4.1326	0.08294	-2.3654
C	7.68117	-1.6806	0.548	H	-6.4859	0.3128	-3.0292
C	6.60108	-2.0606	1.35676	H	-7.3943	2.0316	0.80434
C	5.31629	-1.6342	1.05043	H	-5.0163	1.77649	1.47251
C	3.83223	1.9154	0.81417	H	-0.9808	2.80406	-2.5208
C	-4.3912	0.91188	-0.3995	H	-1.4376	4.97968	-3.5537
C	4.98741	2.56131	0.33821	H	-4.0903	5.95954	-0.317
C	5.64404	3.52236	1.09497	H	-3.615	3.76063	0.726
C	5.16252	3.86972	2.36379	H	-9.9878	1.21007	-2.6752
C	4.01663	3.23934	2.86055	H	-8.4344	1.54016	-3.487
C	3.36945	2.27505	2.08676	H	-8.7852	-0.0943	-2.8576
C	-4.8427	0.50505	-1.6601	H	-1.4521	7.32063	-3.6387
C	-6.1809	0.63607	-2.0408	H	-2.9396	8.26819	-3.905
C	-7.1009	1.18925	-1.1448	H	-2.8224	6.60255	-4.5317
C	-6.6671	1.60463	0.12148	H	4.42464	5.64013	4.29556
C	-5.3336	1.46757	0.48193	H	5.44543	4.36751	5.02271

C	-2.2551	3.11072	-0.8159	H	6.13729	5.97232	4.66735
C	-1.6588	3.49169	-2.0248	H	9.95835	-2.1398	-0.8724
C	-1.9194	4.72884	-2.6161	H	10.8974	-2.2462	0.64017
C	-2.8002	5.62067	-1.9951	H	10.1788	-0.6898	0.14768

Table S16. S_0 optimized geometry of compound **13** at B3LYP/6-31g (d,p) level of theory.

Sum of imaginary frequencies= 1

Total Energy (hartree) = -3710.53555458

Atom	X	Y	Z	Atom	X	Y	Z
C	-2.62094	-2.58046	0.839499	C	7.576258	6.266523	3.016253
C	-1.99527	-3.77857	0.478072	C	6.853682	7.067935	3.901781
C	-2.19876	-1.21724	0.532288	C	5.493069	6.822635	4.094372
C	-3.86446	-2.64911	1.6819	C	4.861565	5.787016	3.407672
C	-2.64223	-5.08472	0.869027	C	-4.31505	7.188264	-1.3434
C	-0.76023	-3.97904	-0.24494	C	-4.76921	8.392622	-1.87814
C	-3.09011	-0.07352	0.284138	C	-5.03575	8.500368	-3.24405
C	-2.26679	1.007139	0.028372	C	-4.84474	7.390625	-4.06891
C	-0.89069	0.503142	0.119714	C	-4.39316	6.185875	-3.53303
N	-0.92308	-0.8348	0.425817	C	-9.3328	0.125902	-1.96331
N	0.193793	-3.04195	-0.44122	C	-10.7053	0.112849	-2.20567
C	1.259844	-3.54294	-1.15682	C	-11.6	-0.17068	-1.1725
C	0.939773	-4.91418	-1.43055	C	-11.1079	-0.44233	0.105138
C	-0.28286	-5.18771	-0.86026	C	-9.73513	-0.43148	0.346243
C	0.332606	1.191552	-0.10017	H	0.061337	-2.05246	-0.12087
C	2.432467	-2.80181	-1.45971	H	1.556467	-5.59384	-1.99922
C	1.480278	0.427752	-0.50485	H	-0.81121	-6.12803	-0.87724
C	2.929085	0.647399	-0.3261	H	1.589775	3.008135	-1.67897
C	3.543909	-0.50629	-0.78524	H	1.782253	5.438842	-1.32158
C	2.45104	-1.39953	-1.20051	H	-0.49684	5.087436	2.299989
N	1.267262	-0.76967	-1.06816	H	-0.69382	2.653907	1.938134
C	0.429114	2.649311	0.101371	H	3.929686	-2.06255	-3.56645
C	3.60778	-3.51159	-2.00761	H	5.858147	-3.24077	-4.55709
C	1.135404	3.462193	-0.80424	H	5.522209	-6.3016	-1.56581

C	1.238765	4.831765	-0.60193	H	3.598617	-5.12425	-0.57552
C	0.656041	5.446041	0.517529	H	-5.14038	-3.65475	0.26635
C	-0.04157	4.636754	1.421844	H	-7.09893	-3.71685	1.746244
C	-0.15994	3.264999	1.217548	H	-4.86189	-1.70215	4.806435
C	4.279202	-2.99104	-3.12644	H	-2.9027	-1.61831	3.309263
C	5.362836	-3.66145	-3.68576	H	-3.49672	-5.46907	-1.0697
C	5.827866	-4.8672	-3.14558	H	-4.49452	-7.63425	-0.43448
C	5.168428	-5.37878	-2.01891	H	-2.93323	-7.18409	3.538275
C	4.077436	-4.72009	-1.4614	H	-1.93272	-5.02324	2.900573
C	-5.06581	-3.238	1.263901	H	-8.26146	-2.74839	3.758062
C	-6.17524	-3.26846	2.1035	H	-7.31421	-1.99396	5.051288
C	-6.12686	-2.72807	3.395774	H	-7.33368	-3.74924	4.874097
C	-4.92899	-2.13565	3.811325	H	-4.84663	-8.86802	2.977617
C	-3.82043	-2.08844	2.967465	H	-5.13792	-9.23689	1.27109
C	-3.3664	-5.84414	-0.05822	H	-3.60958	-9.69142	2.029787
C	-3.93041	-7.06854	0.303071	H	1.833254	7.243681	0.760188
C	-3.78784	-7.57674	1.598997	H	0.312389	7.247196	1.666026
C	-3.05927	-6.81524	2.523052	H	0.306374	7.492281	-0.08544
C	-2.49138	-5.59485	2.165581	H	7.656156	-6.01414	-2.99453
C	-7.32163	-2.80428	4.31615	H	6.648148	-6.44576	-4.37544
C	-4.37943	-8.91087	1.988342	H	7.583933	-4.94828	-4.40662
C	0.782283	6.934658	0.729616	H	5.61254	0.303011	-2.3781
C	6.992179	-5.60375	-3.76182	H	8.009001	-0.18275	-2.10147
C	4.986673	-0.83464	-0.66085	H	7.114978	-2.59574	1.33863
C	5.939379	-0.32607	-1.55554	H	4.725116	-2.06108	1.088961
C	7.293387	-0.61533	-1.40851	H	4.856971	2.342104	-1.26595
C	7.751526	-1.42913	-0.36043	H	5.980469	4.162687	-0.05958
C	6.795876	-1.94292	0.531629	H	3.647194	3.277399	3.437534
C	5.44308	-1.6516	0.384665	H	2.515455	1.466217	2.221096
C	3.59855	1.761445	0.382382	H	-4.39294	-0.98649	-1.88411
C	-4.56064	-0.10647	0.073393	H	-6.81908	-1.03137	-2.31034
C	4.596069	2.534574	-0.23104	H	-7.51577	0.771665	1.526692
C	5.234378	3.564086	0.454755	H	-5.09591	0.76087	1.968614

C	4.902156	3.866975	1.784413	H	-3.93765	2.831362	1.194991
C	3.905717	3.090209	2.399564	H	-4.75648	4.943691	0.245903
C	3.270316	2.060103	1.71531	H	-2.39281	4.268993	-3.27812
C	-5.0779	-0.60556	-1.13219	H	-1.61894	2.130138	-2.34578
C	-6.44813	-0.6191	-1.37651	H	9.582939	-1.9228	-2.31317
C	-7.35923	-0.13299	-0.42461	H	11.98743	-2.41491	-2.04722
C	-6.83922	0.365793	0.780557	H	12.99401	-2.54697	0.224204
C	-5.46869	0.380328	1.023266	H	11.56475	-2.15872	2.223335
C	-2.71498	2.316096	-0.50076	H	9.169591	-1.62702	1.953434
C	-3.60015	3.139084	0.211302	H	7.522695	4.594007	1.667249
C	-4.05165	4.343109	-0.32141	H	8.637591	6.442397	2.864933
C	-3.63747	4.777755	-1.59041	H	7.345847	7.875031	4.436485
C	-2.75116	3.952703	-2.303	H	4.918788	7.445183	4.774824
C	-2.30156	2.748897	-1.7716	H	3.796981	5.621636	3.543824
C	5.575613	4.970201	2.514029	H	-4.08507	7.124195	-0.28408
C	9.195221	-1.73691	-0.20007	H	-4.90651	9.251681	-1.22735
C	-4.11892	6.061191	-2.16005	H	-5.3889	9.438898	-3.66113
C	-8.82133	-0.14653	-0.68287	H	-5.05748	7.459438	-5.13207
C	10.01772	-1.95511	-1.31858	H	-4.27533	5.321485	-4.17957
C	11.37319	-2.24299	-1.16776	H	-8.64757	0.375623	-2.76781
C	11.93809	-2.32202	0.106187	H	-11.077	0.334719	-3.20209
C	11.13419	-2.10877	1.227191	H	-12.6696	-0.17939	-1.36094
C	9.779374	-1.81862	1.075619	H	-11.7943	-0.67208	0.915339
C	6.944907	5.229439	2.331732	H	-9.36164	-0.67011	1.337641

Table S17. S_0 optimized geometry of compound **14** at B3LYP/6-31g (d,p) level of theory.

Sum of imaginary frequencies= 1

Total Energy (hartree) = -4069.28918546

Atom	X	Y	Z	Atom	X	Y	Z
C	2.87974	-1.0966	0.30935	C	-3.4829	2.39293	2.38634
C	2.46105	-2.4127	0.08948	C	-4.3128	3.27063	3.01722
C	2.13087	0.13424	0.07564	S	-5.795	3.48849	2.13929
C	4.24851	-0.8695	0.88756	C	-5.2814	2.37242	0.91667

C	3.43162	-3.5394	0.34709	C	2.59857	4.65386	-0.7929
C	1.17611	-2.8954	-0.3634	C	2.48931	5.76441	-1.5775
C	2.69451	1.4084	-0.3874	S	1.27634	5.55998	-2.8018
C	1.62746	2.27848	-0.5122	C	0.9206	3.96092	-2.242
C	0.43489	1.52582	-0.1083	C	5.10209	2.32847	-0.0856
N	0.80741	0.2458	0.22359	C	6.26892	2.49348	-0.7734
N	0.02485	-2.1875	-0.3487	S	6.15179	1.86057	-2.385
C	-1.0351	-2.9301	-0.8239	C	4.50927	1.3749	-2.1189
C	-0.4929	-4.2132	-1.1672	H	0.0113	-1.1763	-0.0689
C	0.85123	-4.2007	-0.8706	H	-1.0531	-5.0291	-1.5985
C	-0.9233	1.94473	-0.0587	H	1.55317	-5.0087	-1.0046
C	-2.3762	-2.465	-0.8629	H	0.24594	3.73618	1.61145
C	-1.9452	0.94113	-0.1752	H	-0.3549	6.10538	1.9432
C	-3.3317	0.8711	0.32623	H	-3.5037	5.71018	-0.9485
C	-3.7741	-0.4098	0.02983	H	-2.9017	3.34292	-1.2807
C	-2.6345	-1.0842	-0.6112	H	-2.7632	-4.9553	0.22348
N	-1.6117	-0.2202	-0.7561	H	-4.5663	-6.5501	-0.2991
C	-1.2748	3.36397	0.13216	H	-6.2663	-3.7291	-3.0527
C	-3.4648	-3.4284	-1.128	H	-4.4543	-2.1371	-2.5393
C	-0.5667	4.17149	1.03903	H	3.42317	0.00643	2.67187
C	-0.9116	5.50546	1.22786	H	5.60768	0.37314	3.76196
C	-1.9689	6.08797	0.51683	H	7.58461	-1.271	0.3245
C	-2.6779	5.28213	-0.3859	H	5.40995	-1.6571	-0.7484
C	-2.3434	3.94656	-0.5728	H	3.13161	-3.5345	2.47924
C	-3.5176	-4.6895	-0.5096	H	4.66391	-5.4158	2.91197
C	-4.5434	-5.5856	-0.8	H	5.48083	-5.7181	-1.2909
C	-5.5522	-5.262	-1.7152	H	3.95119	-3.8304	-1.722
C	-5.4991	-4.0035	-2.3331	H	8.0049	0.32943	3.7335
C	-4.4829	-3.1014	-2.0427	H	8.7787	0.36123	2.14225
C	4.33576	-0.2792	2.15635	H	8.60242	-1.1654	3.00349
C	5.57164	-0.0723	2.77062	H	6.63804	-7.189	0.2055
C	6.76277	-0.4283	2.13116	H	6.88345	-6.6019	1.85616
C	6.67396	-0.9985	0.85245	H	5.57853	-7.7344	1.51094

C	5.44399	-1.2212	0.24313	H	-1.9857	7.92152	1.66594
C	3.64497	-4.0115	1.64979	H	-3.4017	7.70587	0.6231
C	4.51209	-5.0737	1.89089	H	-1.848	8.16133	-0.0775
C	5.19023	-5.7113	0.8423	H	-7.6092	-5.8959	-1.5314
C	4.96794	-5.2445	-0.4574	H	-6.878	-6.283	-3.0874
C	4.10277	-4.1766	-0.7032	H	-6.4542	-7.2282	-1.6509
C	8.10482	-0.2121	2.78877	H	-4.2833	-2.3979	2.03277
C	6.12209	-6.8684	1.1147	H	-6.7712	-3.1533	2.4563
C	-2.3219	7.54394	0.69602	H	-6.5074	-0.0253	-0.8543
C	-6.6786	-6.2211	-2.0125	H	-2.51	2.10941	2.76904
C	-5.046	-1.0235	0.46123	H	-4.149	3.79782	3.94641
C	-4.0299	1.86256	1.16405	H	-5.9212	2.17341	0.07086
C	4.0747	1.67979	-0.8532	H	3.29735	4.57268	0.03004
C	1.69018	3.60163	-1.1616	H	3.04556	6.68876	-1.5117
C	-5.1439	-2.0219	1.49259	H	0.1661	3.36797	-2.7381
C	-6.4226	-2.4313	1.73137	H	4.96759	2.63055	0.94596
S	-7.5555	-1.6165	0.69897	H	7.19205	2.93918	-0.4308
C	-6.2809	-0.7121	-0.0516	H	3.94588	0.90369	-2.9119

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