Impact of Phenothiazine-to-Phenoxazine Replacement in Hexaphyrin Frameworks on Structural, Spectroscopic, and Redox Properties

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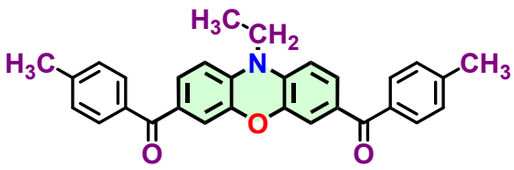
Experimental Section

- 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. Basic alumina and silica gel (60-120 mesh) column chromatographic methods were used for purification purposes. Reported methods were used for the synthesis of compounds**, 3a-b, 4a, 5a** and **6a**.[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.
- 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] where as in case of solid absolute quantum yield has been calculated using absolute method.
- **Differential pulse voltammetry (DPV)** studies were performed with BAS electrochemical system with the three-electrode configuration comprising of a saturated calomel electrode (reference electrode), glassy carbon (working electrode), (auxiliary electrode) and 10^{-3} M of the analyte. Bruker maXis Impact, Q-TOF, and MALDI -TOF mass spectrometer instruments were used for recording HR mass spectra.
- **X-ray Crystallography data for the compound 2a**

  Single crystals of all compounds were mounted on a Cryoloop with a drop of Paratone oil and positioned in the cold nitrogen stream on a Rigaku Saturn724+ (2x2 bin mode) diffractometer for **2a.** The data collections were performed at 150 K using a graphite mono chromated MoKα (λ = 0.71073) radiation source for compounds **2a**. The data were reduced using Crysalis Pro Red 171.41_64.93a software. The structures were solved using Olex21 with the ShelXT2 structure solution program using intrinsic phasing and refined with the SHELXL3 refinement package using least-squares minimization. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.
- **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 in conjunction with basis set 6-31G(d,p)[5] was implemented to optimize the structure of macrocycles **2a** 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) 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 **4b**

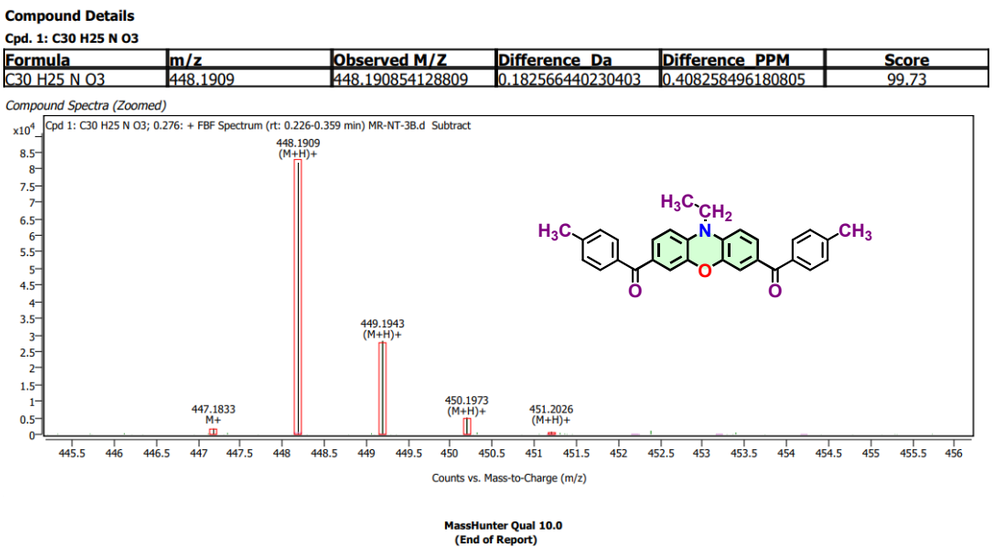


Figure S1. HR mass spectrum of compound **4b.**

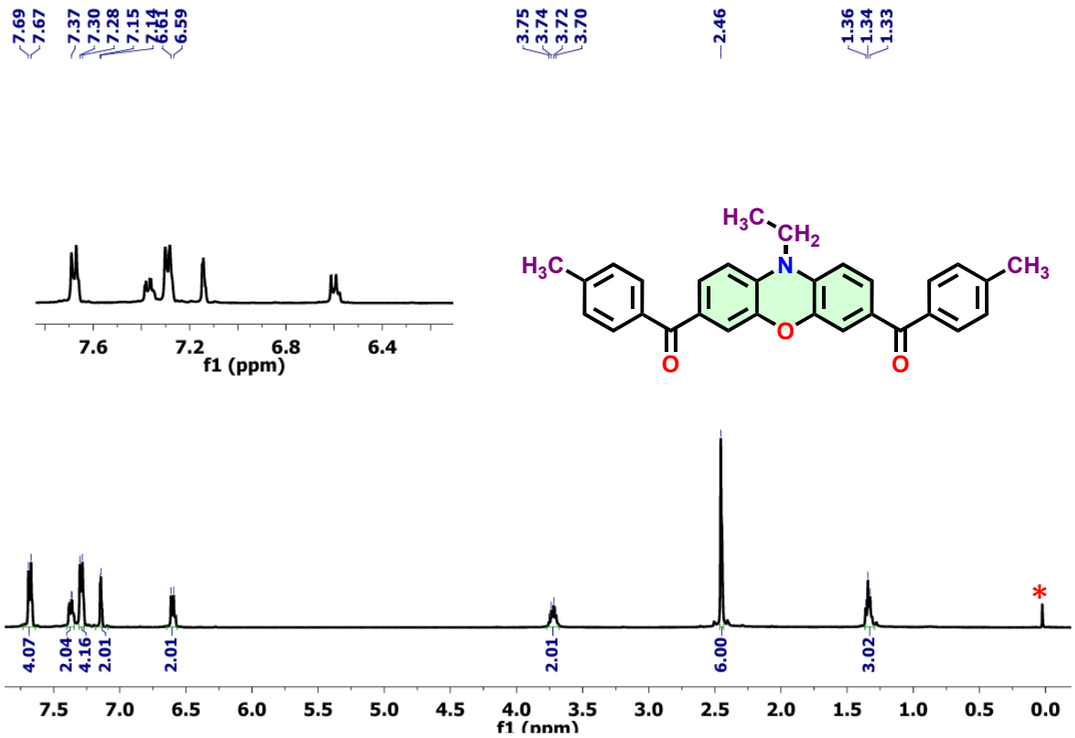


Figure S2. ^{1}H NMR spectrum of the compound **4b** recorded in $CDCl_3$ on 400 MHz NMR instrument. Expansion of aromatic region is given as an inset. Note: Peaks marked with asterisk (*) are due to residual solvents.

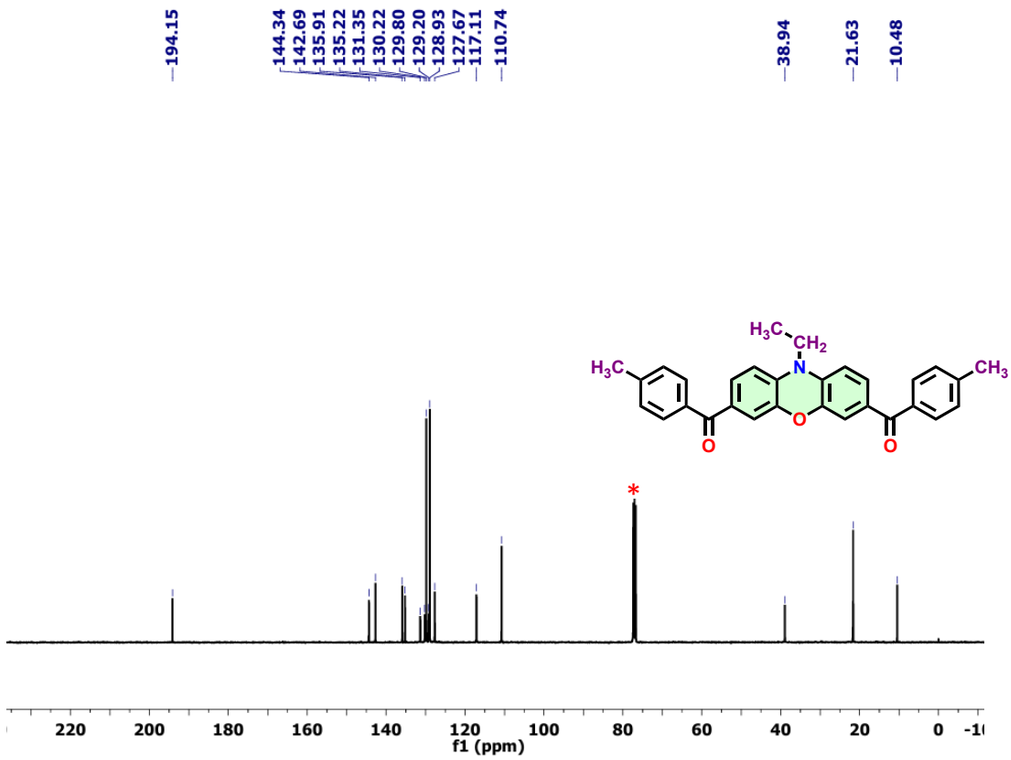
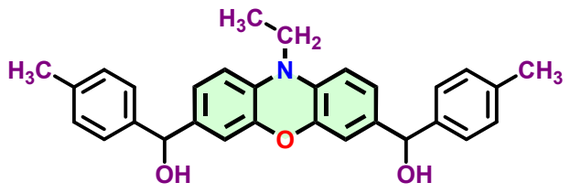


Figure S3. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **4b** recorded in $CDCl_3$ on 100.06 MHz NMR instrument; Note: Peaks marked with asterisk (*) are due to residual solvents.



Compound **5b**

Compound Details

Cpd. 1: C30 H29 N O3

Formula	m/z	Observed M/Z	Difference_Da	Difference_PPM	Score
C30 H29 N O3	452.2214	452.221391165466	-0.199258111877043	-0.441603725532579	94.87

Compound Spectra (Zoomed)

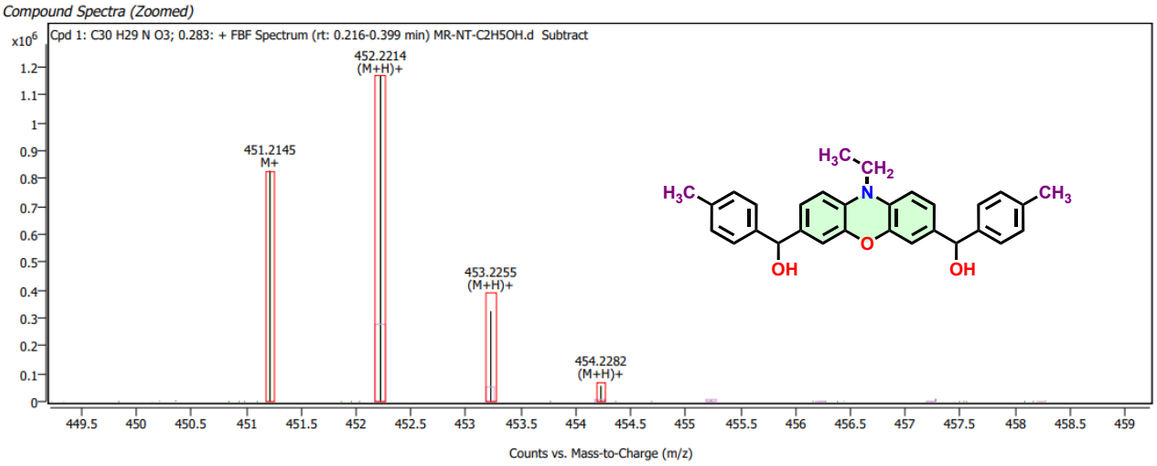


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Figure S4. HR mass spectrum of compound **5b.**

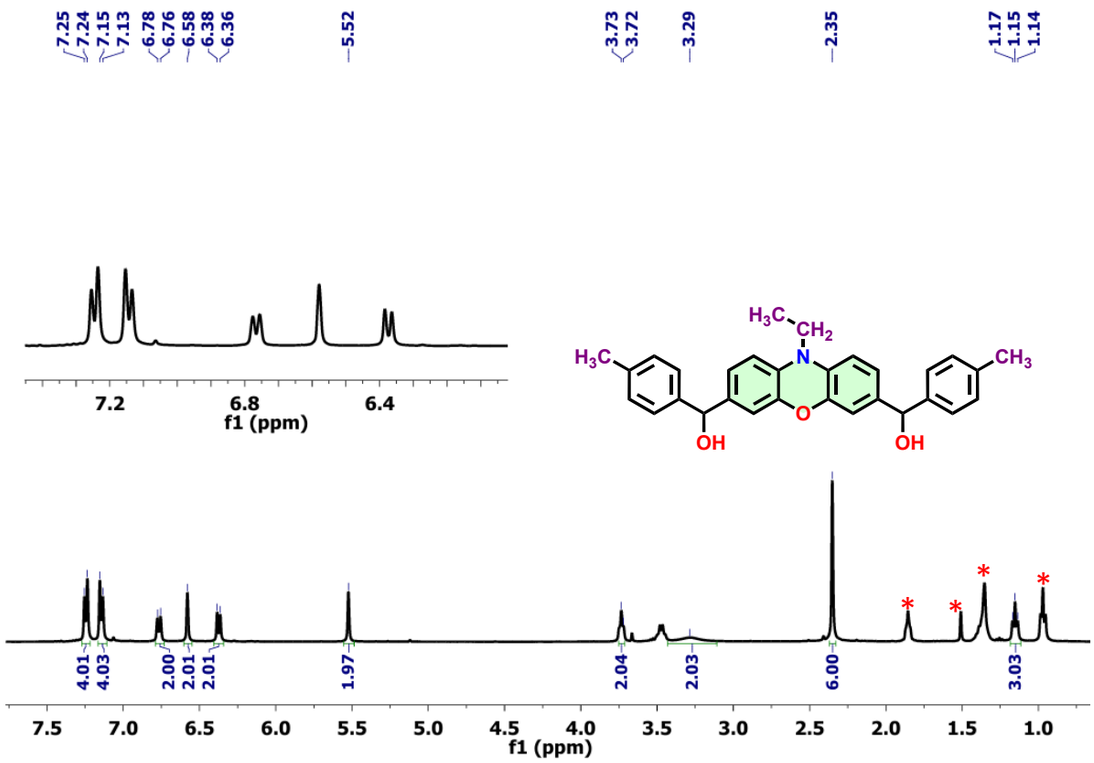


Figure S5. ^{1}H NMR spectrum of the compound **5b** recorded in $CDCl_3$ on 500 MHz NMR instrument. Expansion of aromatic region is given as an inset. Note: Peaks marked with asterisk (*) are due to residual solvents.

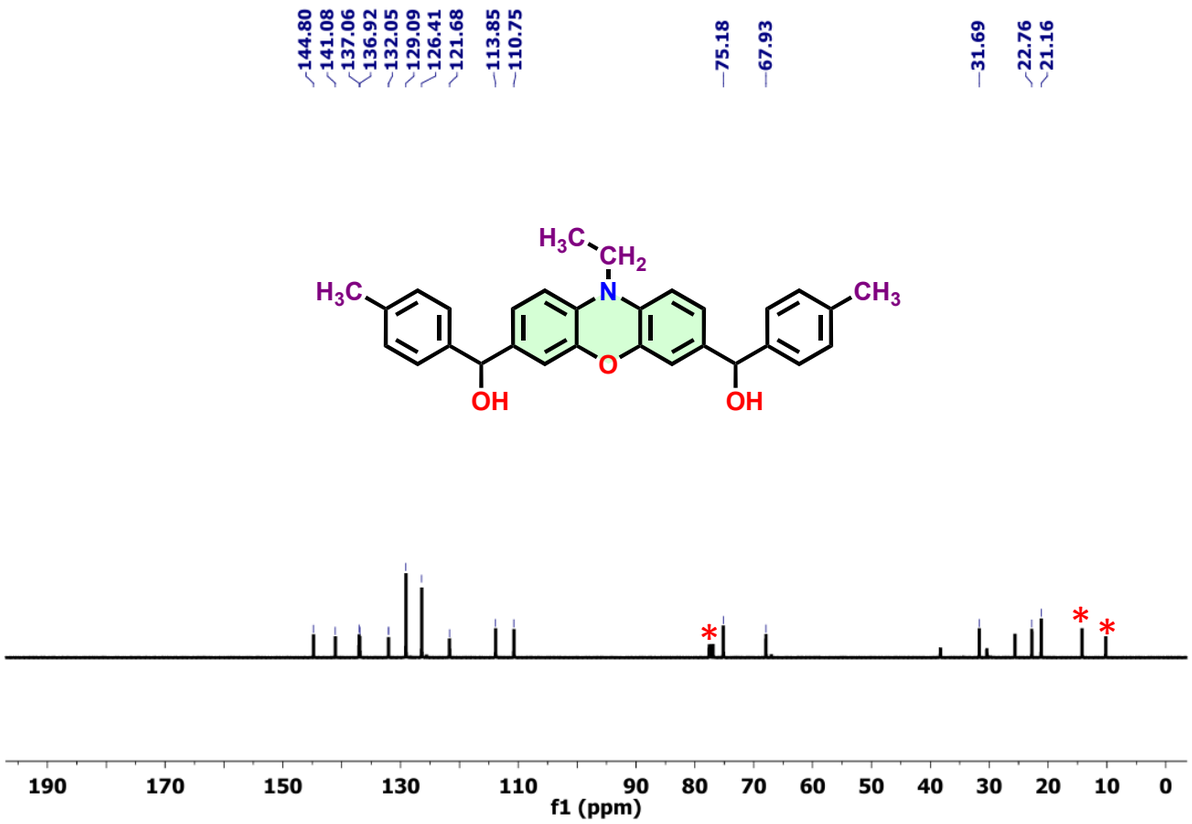
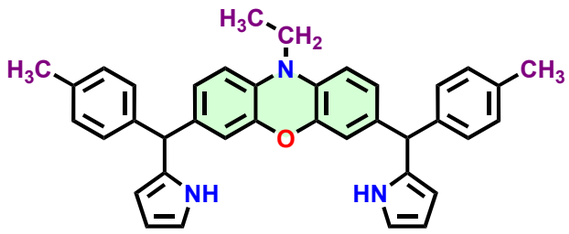


Figure S6. $^{13}C\{1H\}$ NMR spectrum of the compound **5b** recorded in $CDCl_3$ on 100.06 MHz NMR instrument; Note: Peaks marked with asterisk (*) are due to residual solvents like *n*-hexane.



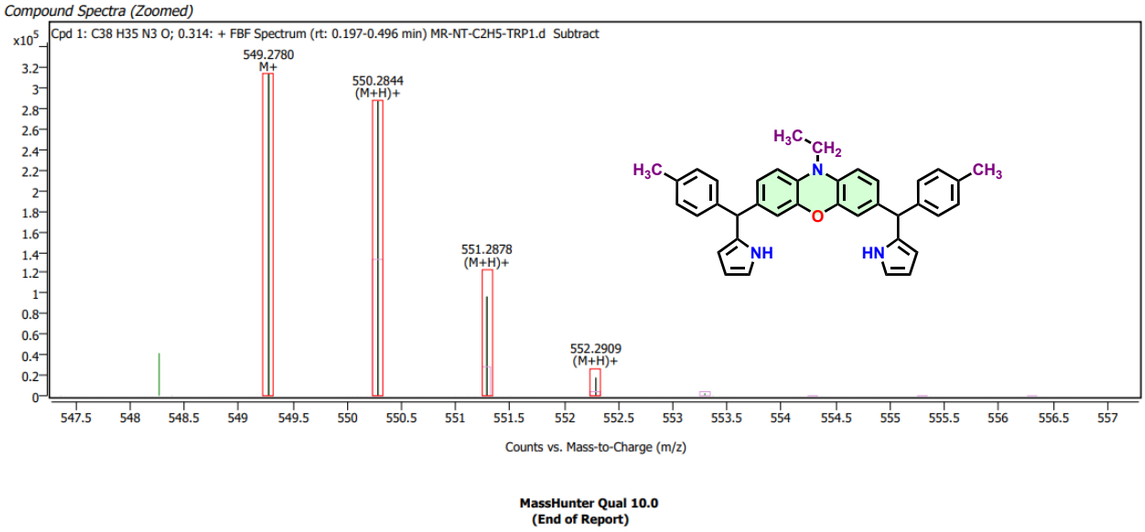
Compound **6b**

Compound Details

Cpd. 1: C38 H35 N3 O

Formula	m/z	Observed M/Z	Difference_Da	Difference_PPM	Score
C38 H35 N3 O	550.2844	550.284424275271	-0.22280649750428	-0.40563520171565	91.12

Compound Spectra (Zoomed)



MassHunter Qual 10.0
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Figure S7. HR mass spectrum of compound **6b.**

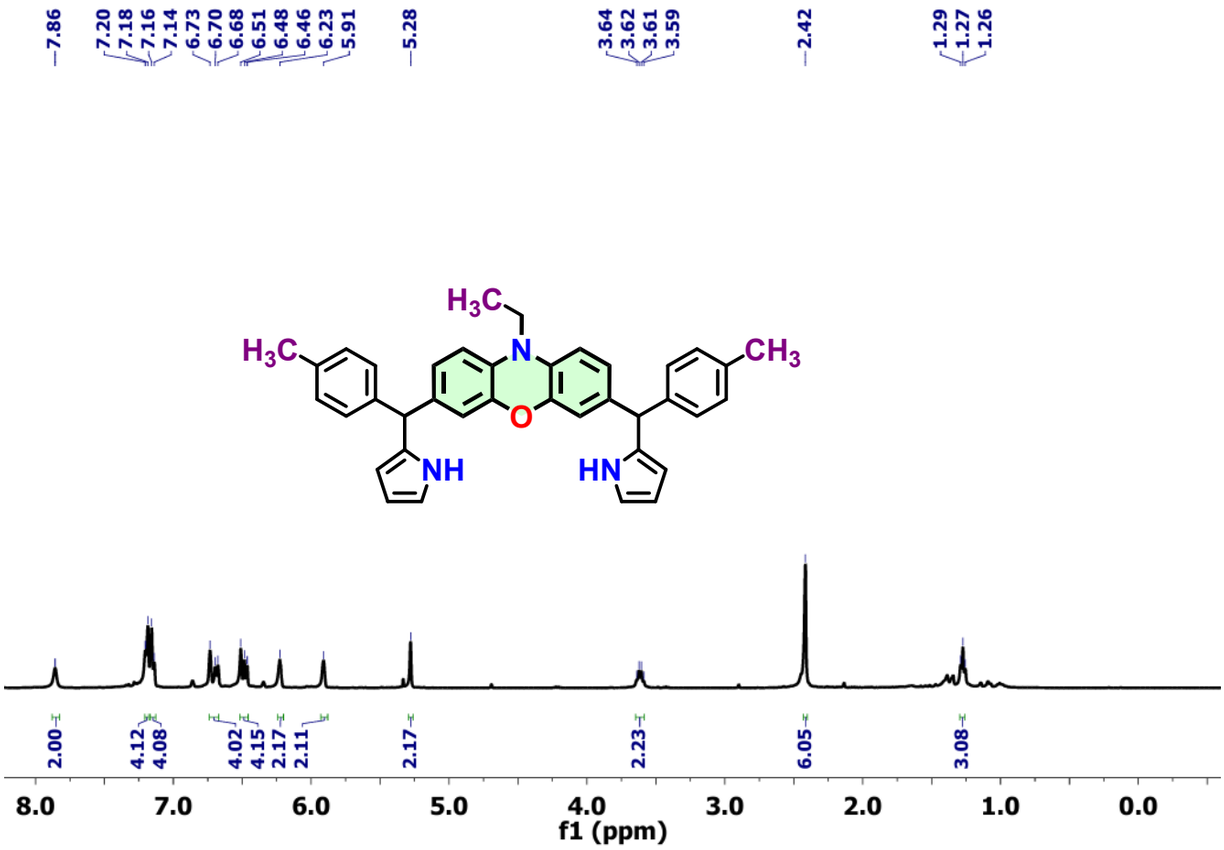


Figure S8. ^{1}H NMR spectrum of the compound **6b** recorded in $CDCl_3$ on 500 MHz NMR instrument. Expansion of aromatic region is given as an inset. Note: Peaks marked with asterisk (*) are due to residual solvents.

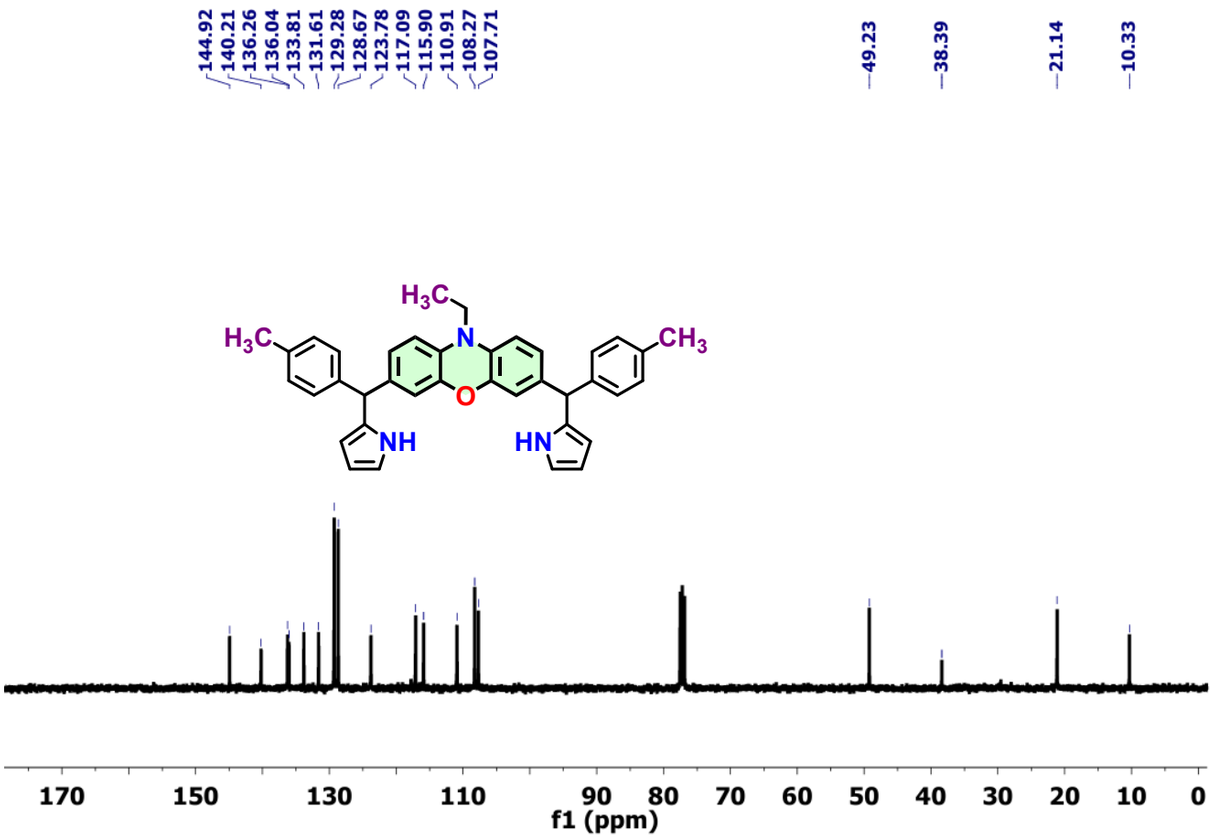
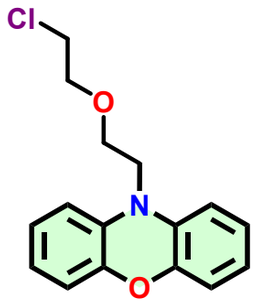


Figure S9. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **6b** recorded in $CDCl_3$ on 100.06 MHz NMR instrument; Note: Peaks marked with asterisk (*) are due to residual solvents.



Compound **3c**

Compound Details

Cpd. 1: C16 H16 Cl N O2

Formula	m/z	Observed M/Z	Difference_Da	Difference_PPM	Score
C16 H16 Cl N O2	290.0939	290.093943773036	-0.280485321184187	-0.970245508849051	97.99

Compound Spectra (Zoomed)

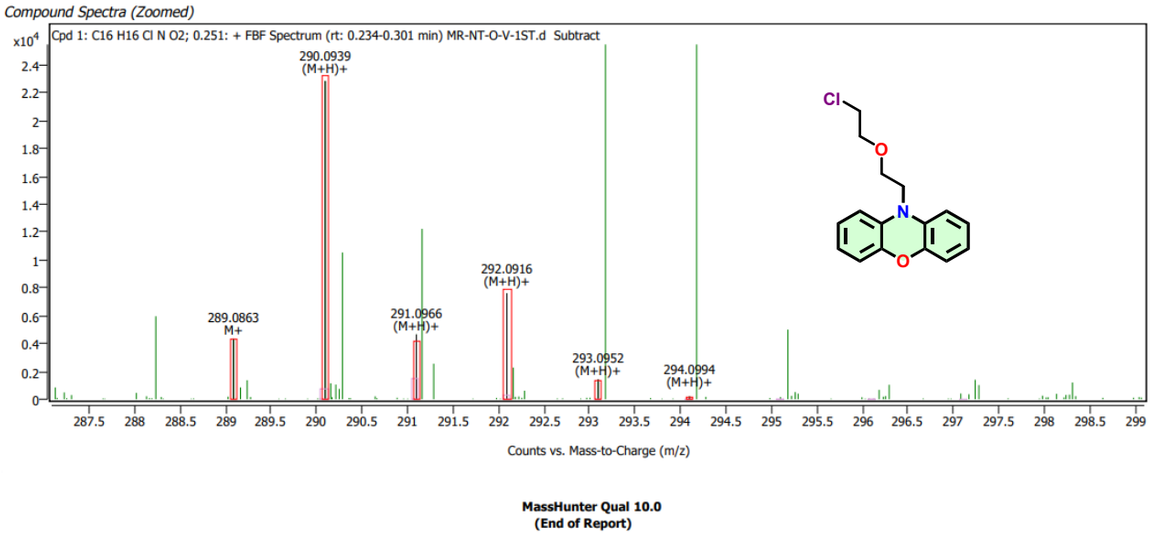


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Figure S10. HR mass spectrum of compound **3c.**

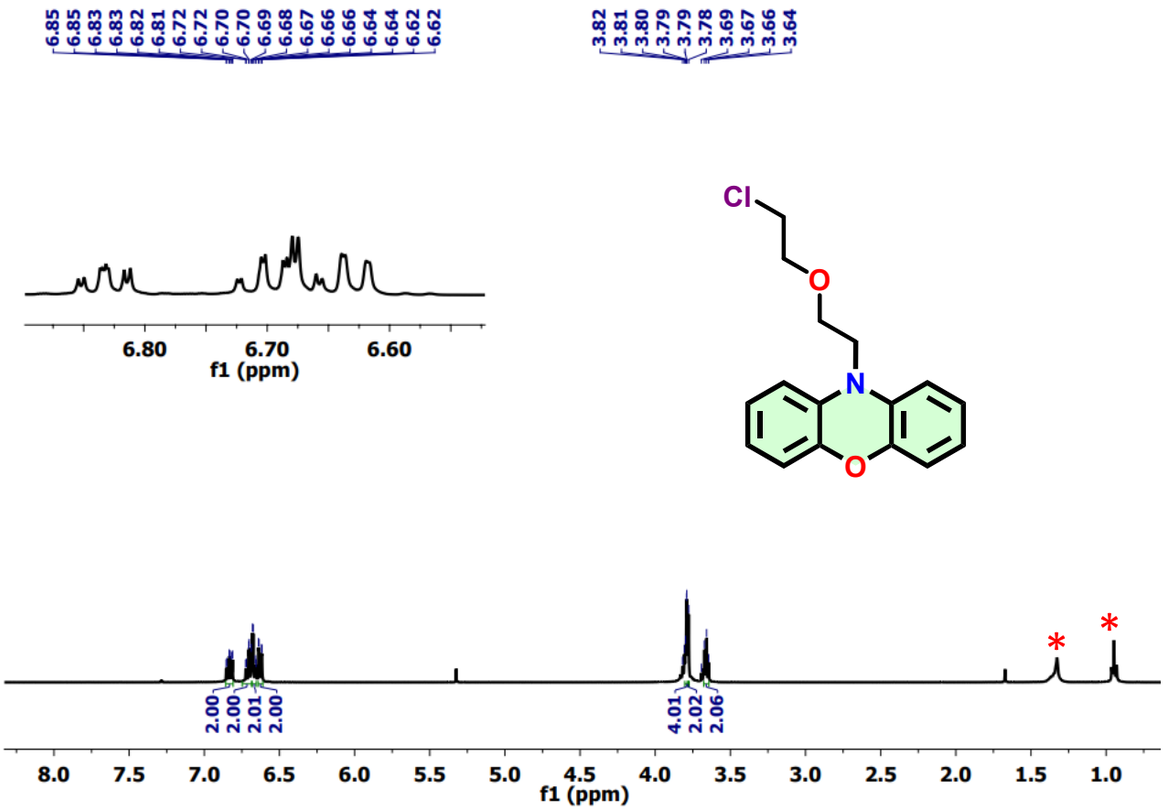


Figure S11. ^{1}H NMR spectrum of the compound **3c** recorded in $CDCl_3$ on 500 MHz NMR instrument. Expansion of aromatic region is given as an inset. Note: Peaks marked with asterisk (*) are due to residual solvents.

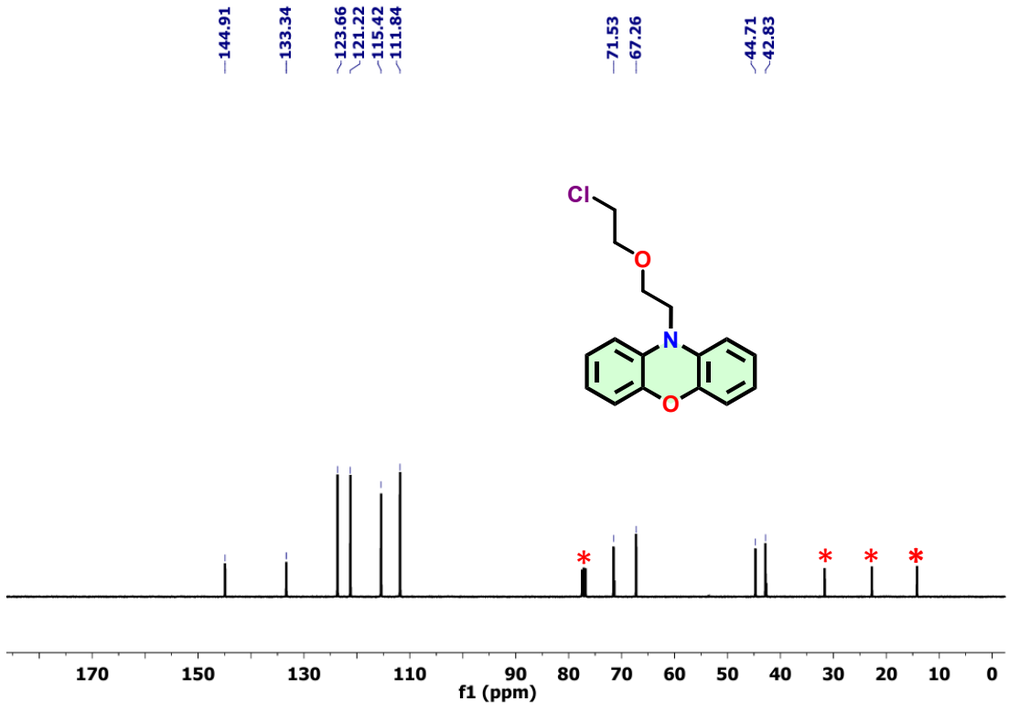
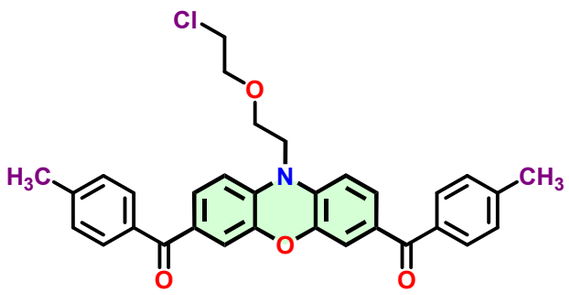


Figure S12. $^{13}C\{1H\}$ NMR spectrum of the compound **4c** recorded in $CDCl_3$ on 100.06 MHz NMR instrument; Note: Peaks marked with asterisk (*) are due to residual solvents like *n*-hexane.



Compound **4c**

Compound Details

Cpd. 1: C32 H29 Cl N O4

Formula	m/z	Observed M/Z	Difference_Da	Difference_PPM	Score
C32 H29 Cl N O4	526.1779	526.177874192261	-0.110539660113318	-0.210080149178974	98.95

Compound Spectra (Zoomed)

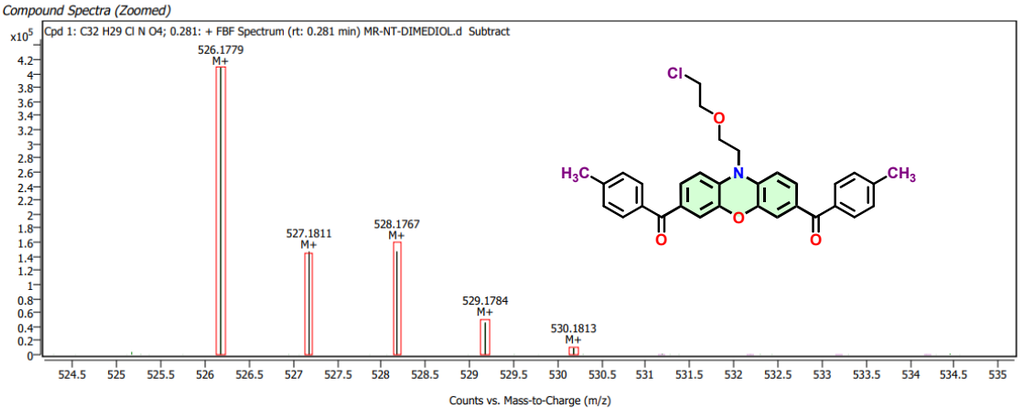


Figure S13. HR mass spectrum of compound **4c.**

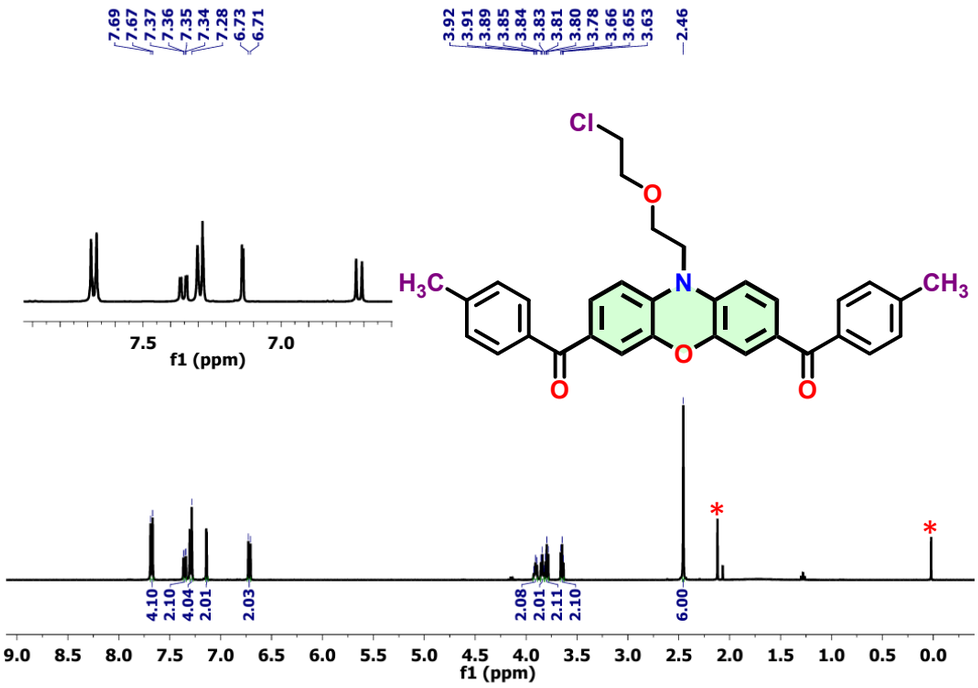


Figure S14. ^{1}H NMR spectrum of the compound **4c** recorded in $CDCl_3$ on 500 MHz NMR instrument. Expansion of aromatic region is given as an inset. Note: Peaks marked with asterisk (*) are due to residual solvents.

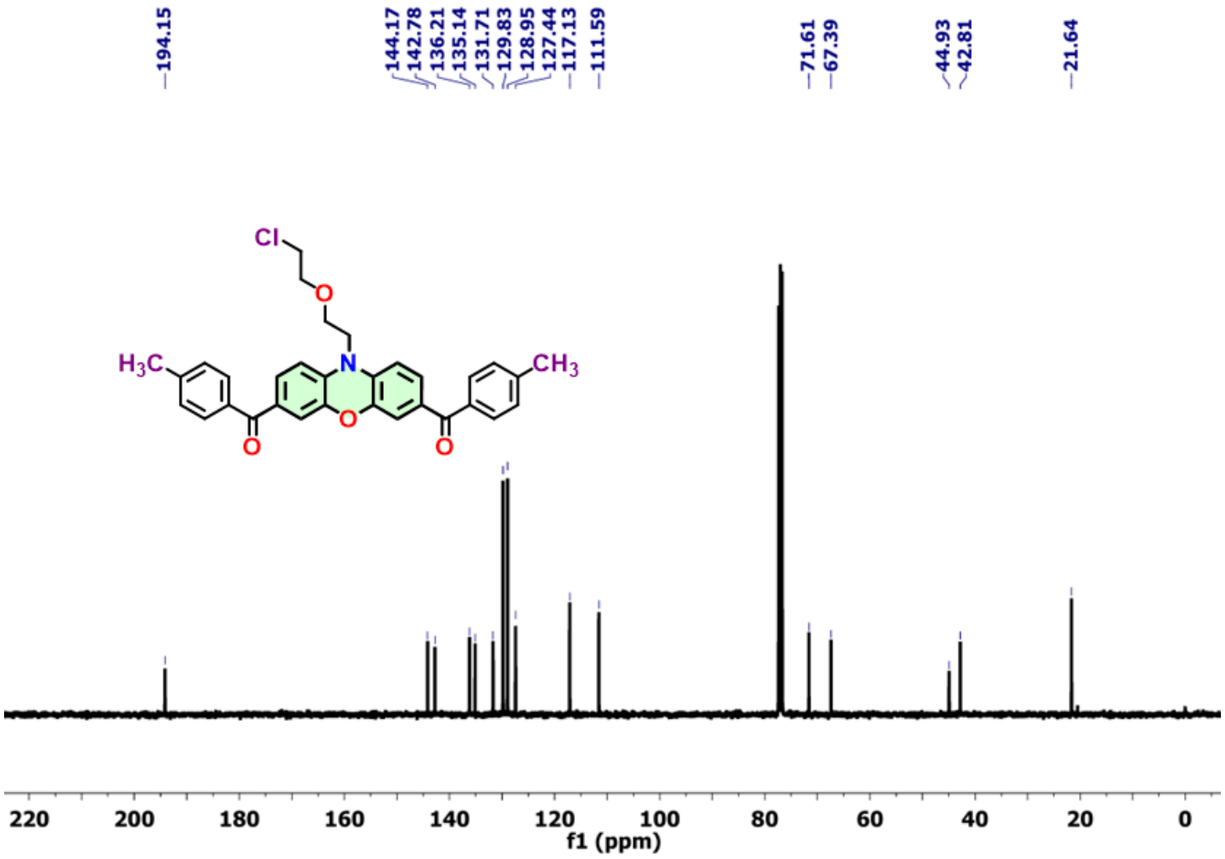
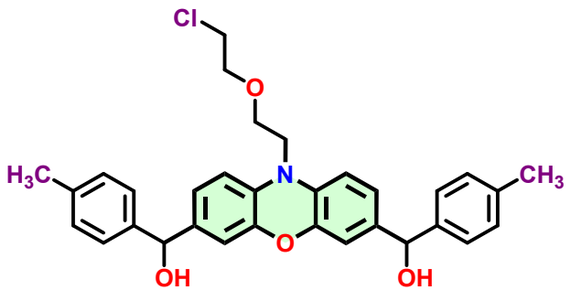


Figure S15. $^{13}C\{1H\}$ NMR spectrum of the compound **4c** recorded in $CDCl_3$ on 100.06 MHz NMR instrument; Note: Peaks marked with asterisk (*) are due to residual solvents.



Compound **5c**

Compound Details

Cpd. 1: C32 H31 Cl N O3

Formula	m/z	Observed M/Z	Difference_Da	Difference_PPM	Score
C32 H31 Cl N O3	512.1986	512.198557144512	0.149667709820278	0.292206032753093	98.42

Compound Spectra (Zoomed)

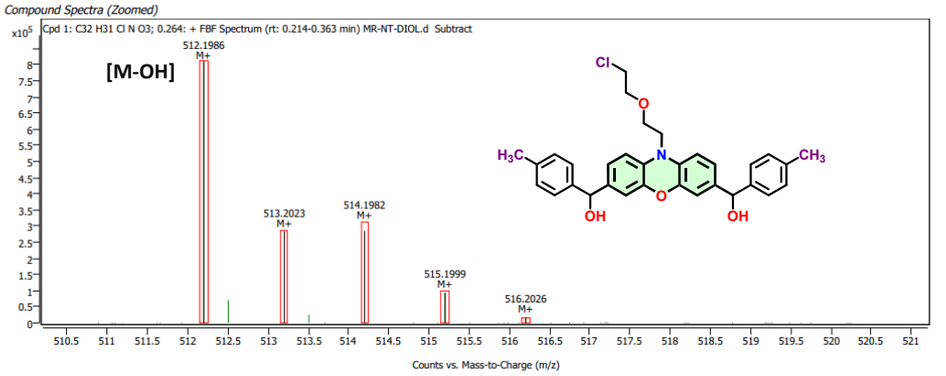


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Figure S16. HR mass spectrum of compound **5c.**

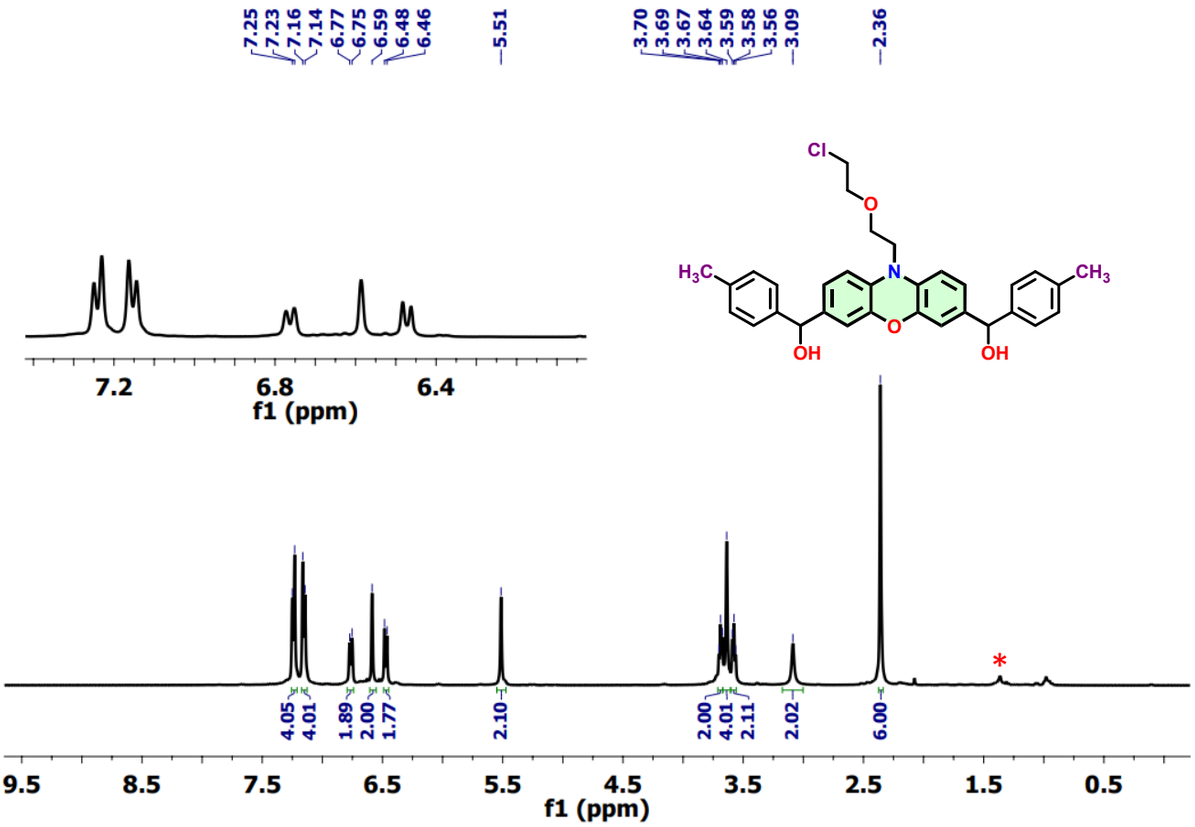


Figure S17. ^{1}H NMR spectrum of the compound **5c** recorded in $CDCl_3$ on 500 MHz NMR instrument. Expansion of aromatic region is given as an inset. Note: Peaks marked with asterisk (*) are due to residual solvents.

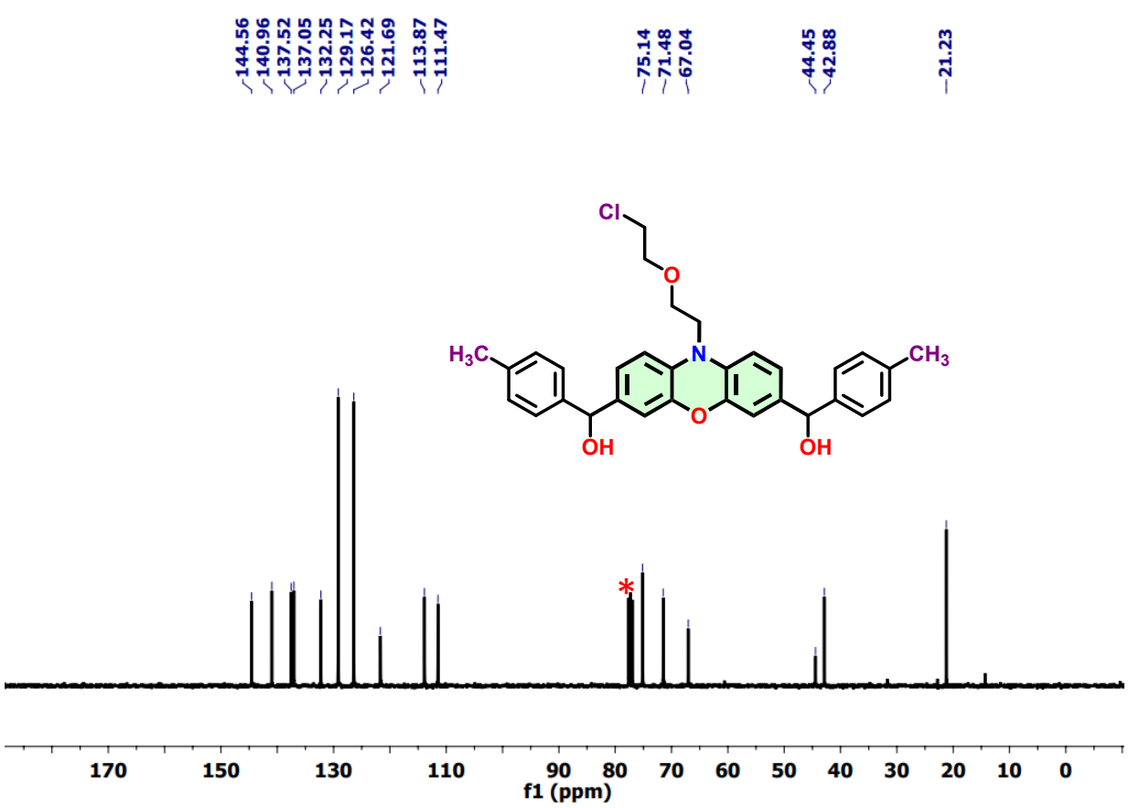
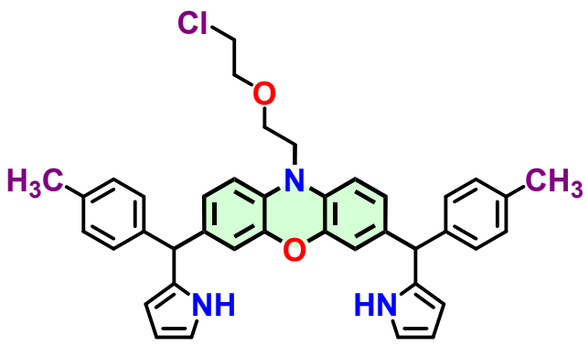


Figure S18. $^{13}C\{1H\}$ NMR spectrum of the compound **5c** recorded in $CDCl_3$ on 100.06 MHz NMR instrument; Note: Peaks marked with asterisk (*) are due to residual solvents.



Compound Details

Cpd. 1: C40 H38 Cl N3 O2

Formula	m/z	Observed M/Z	Difference_Da	Difference_PPM	Score
C40 H38 Cl N3 O2	627.2641	627.264112349485	0.0551230849623607	0.0878784286334363	94.33

Compound Spectra (Zoomed)

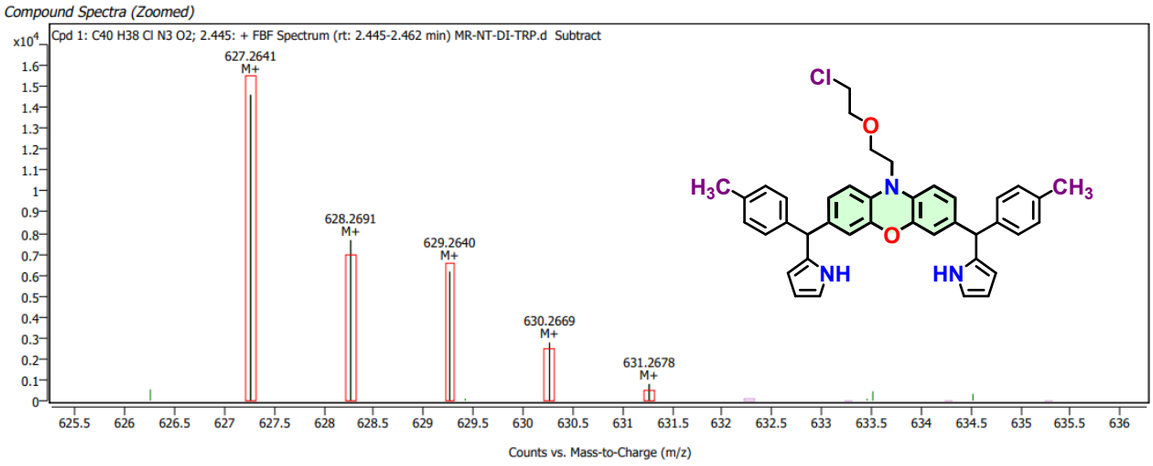


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Figure S19. HR mass spectrum of compound **6c.**

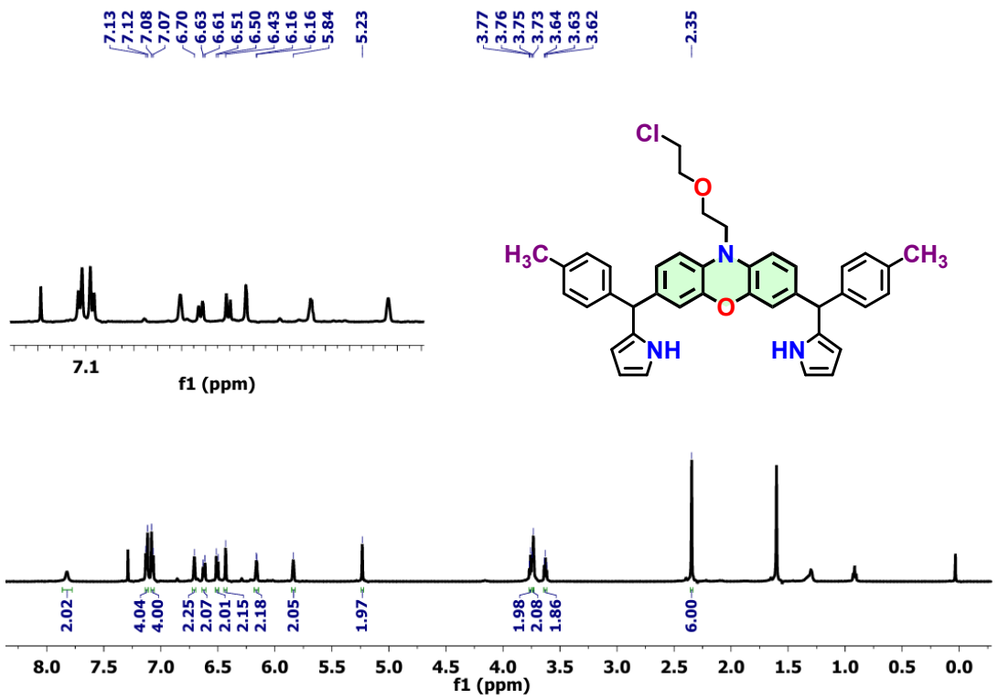


Figure S20. ^{1}H NMR spectrum of the compound **6c** recorded in $CDCl_3$ on 500 MHz NMR instrument. Expansion of aromatic region is given as an inset. Note: Peaks marked with asterisk (*) are due to residual solvents.

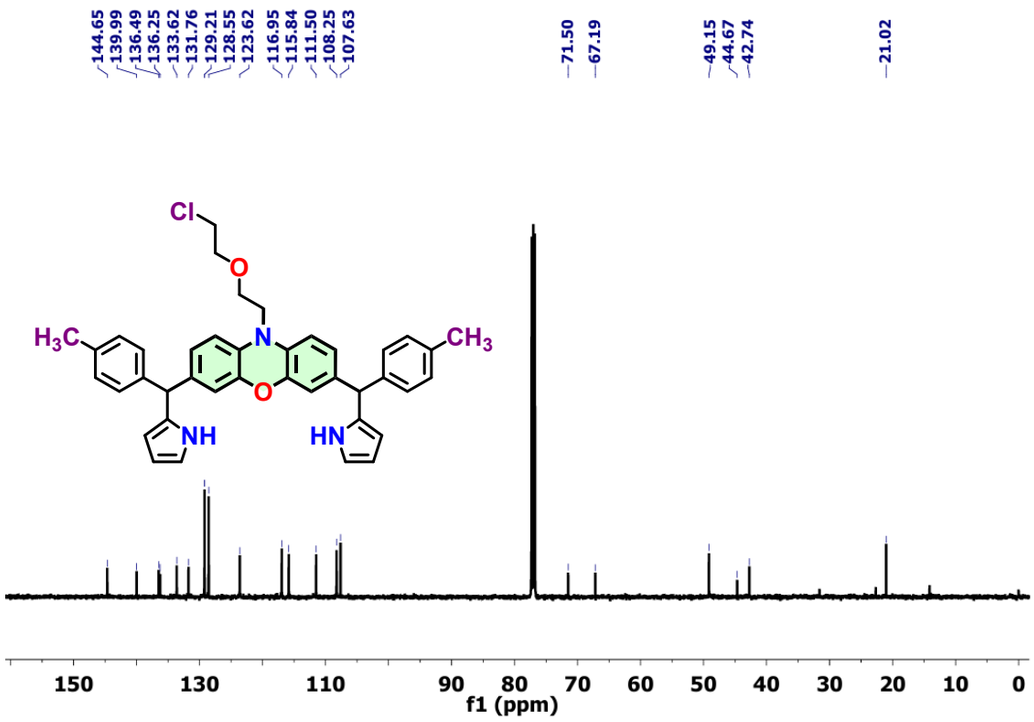
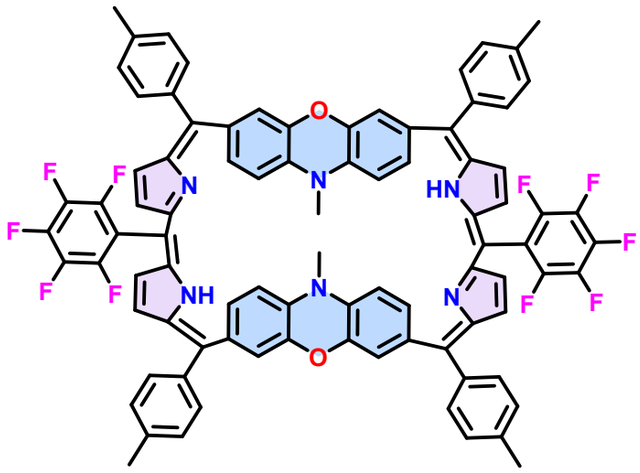


Figure S21. $^{13}C\{1H\}$ NMR spectrum of the compound **6c** recorded in $CDCl_3$ on 100.06 MHz NMR instrument; Note: Peaks marked with asterisk (*) are due to residual solvents.



Compound **2a**

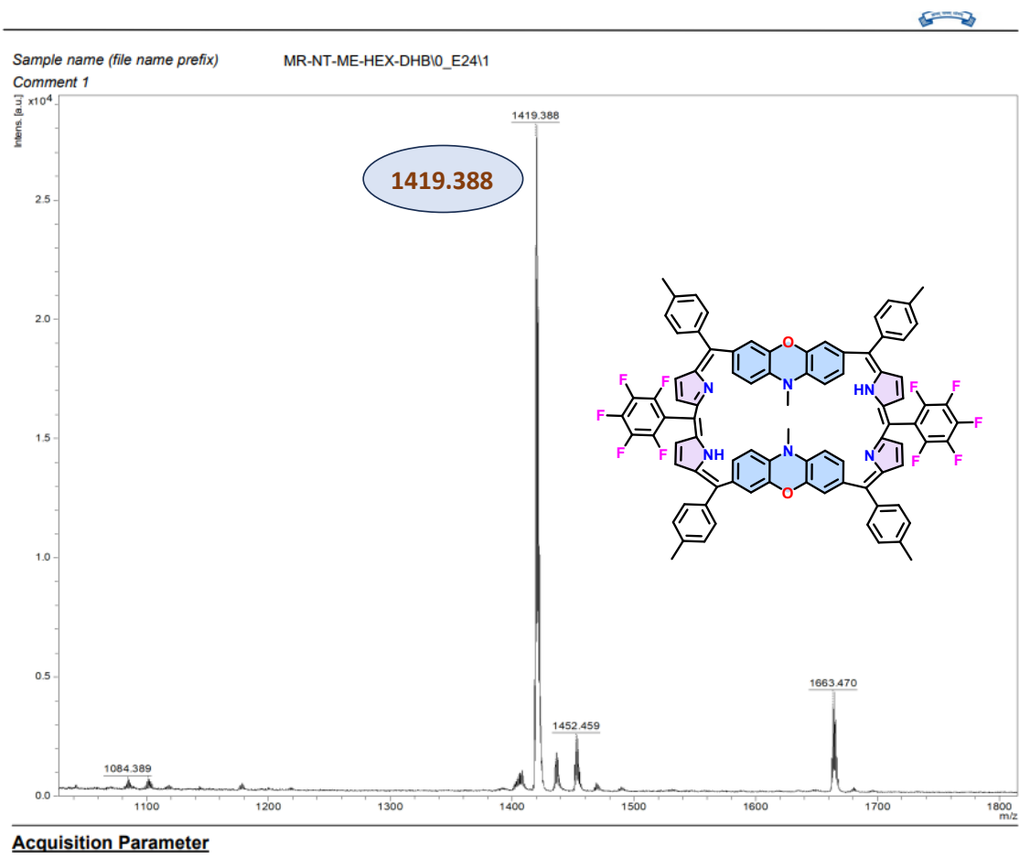


Figure S22. HR mass spectrum of compound **2a.**

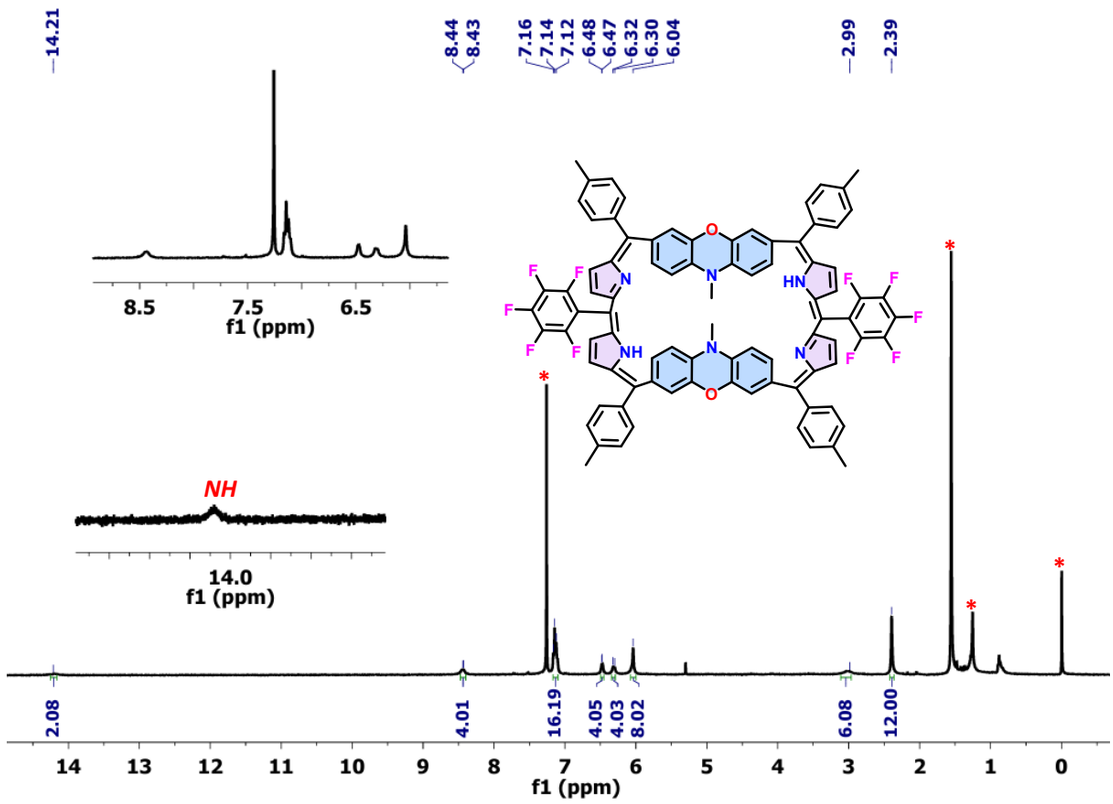


Figure S23. ^{1}H NMR spectrum of the compound **2a** recorded in $CDCl_3$ on 500 MHz NMR instrument. Expansion of aromatic region is given as an inset. Note: Peaks marked with asterisk (*) are due to residual solvents.

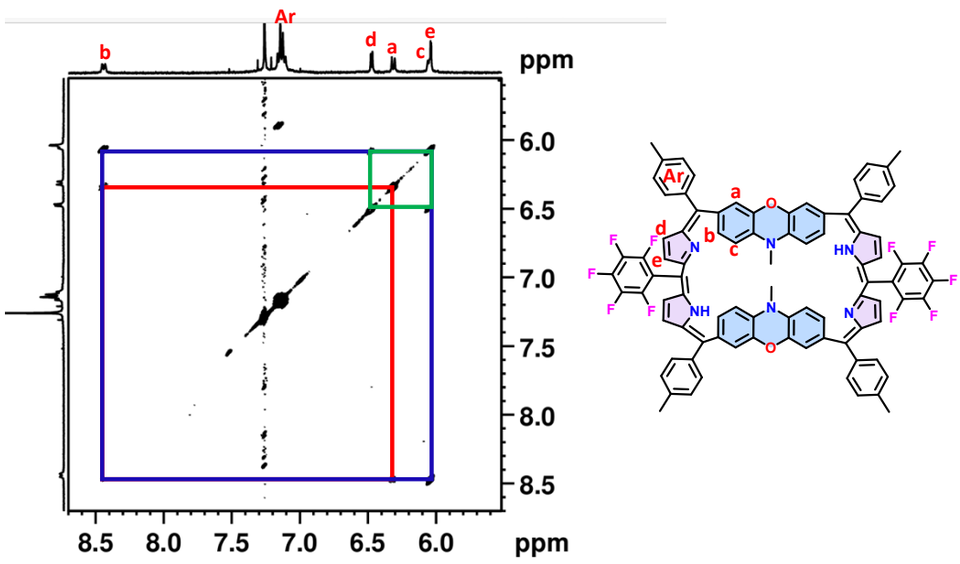
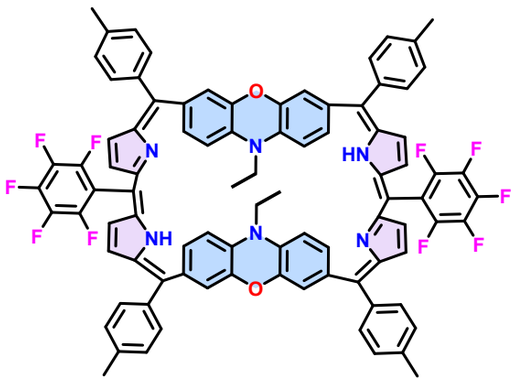


Figure S25. ^{1}H-^{1}H COSY of compound **2a** recorded in $CDCl_3$ at 25 °C.



Compound **2b**

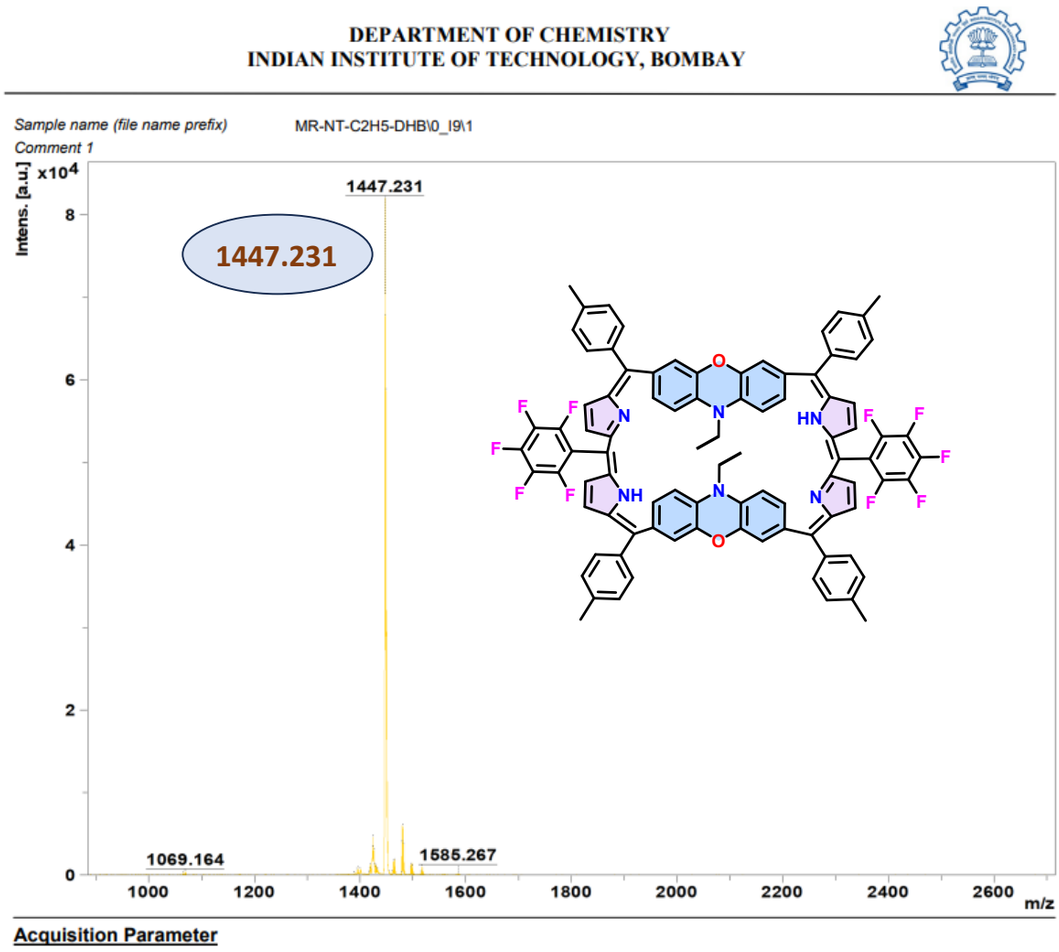


Figure S25. HR mass spectrum of compound **2b.**

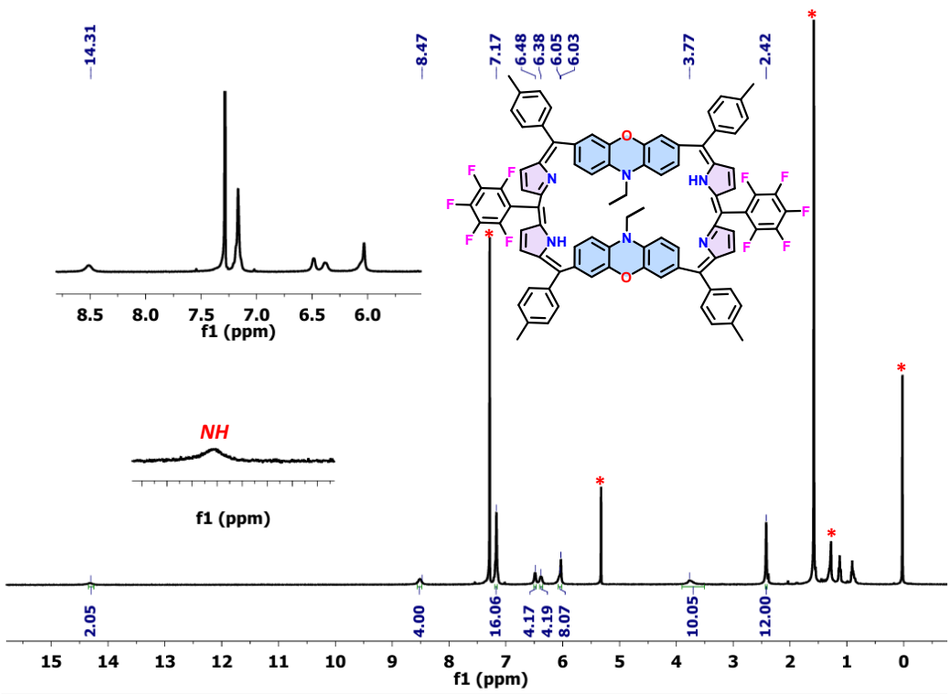


Figure S26. ^{1}H NMR spectrum of the compound **2b** recorded in $CDCl_3$ on 500 MHz NMR instrument. Expansion of aromatic region is given as an inset. Note: Peaks marked with asterisk (*) are due to residual solvents.

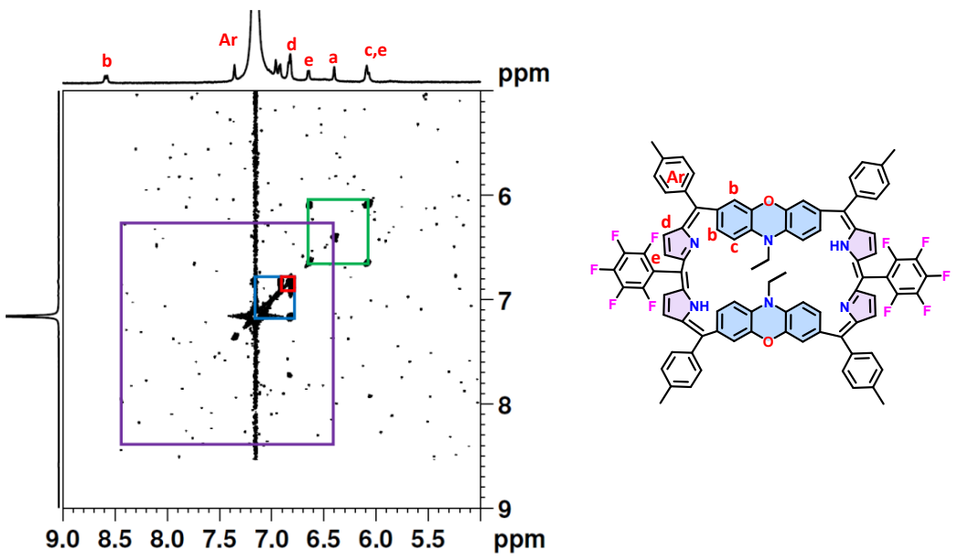
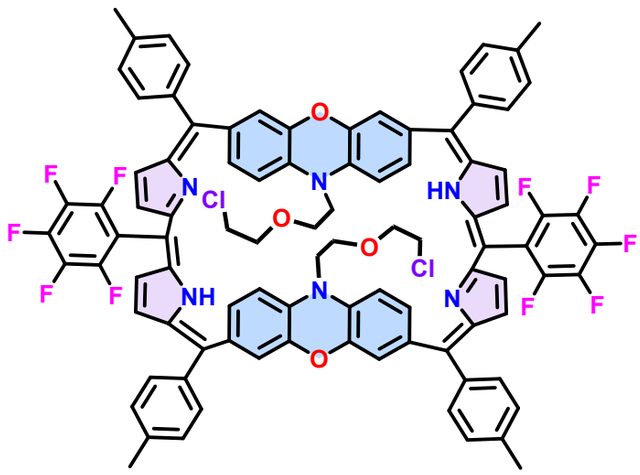


Figure S27. ^{1}H-^{1}H COSY of compound **2b** recorded in $CDCl_3$ at 25 °C.



Compound **2c**

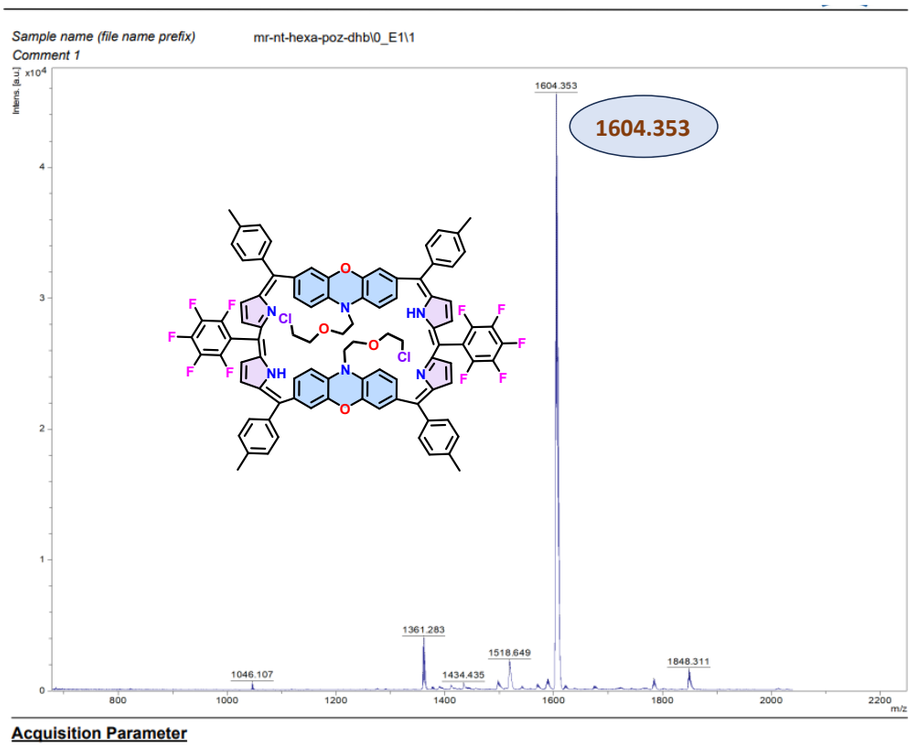


Figure S28. HR mass spectrum of compound **2c.**

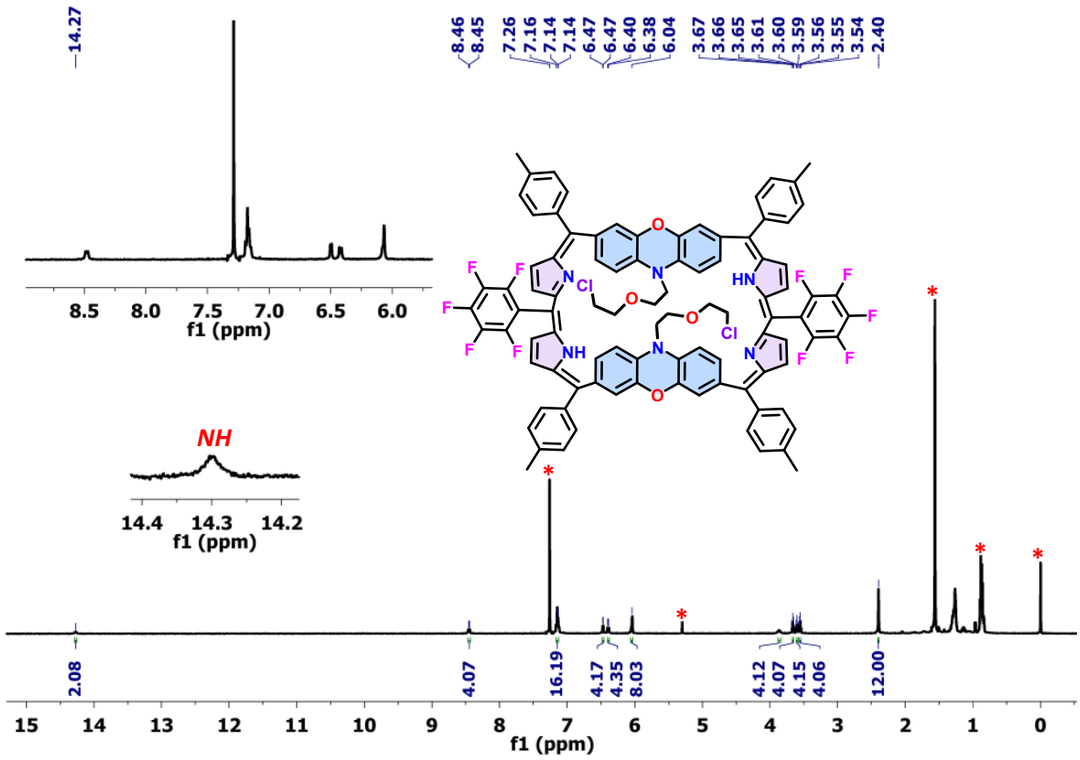


Figure S29. ^{1}H NMR spectrum of the compound **2c** recorded in $CDCl_3$ on 500 MHz NMR instrument. Expansion of aromatic region is given as an inset. Note: Peaks marked with asterisk (*) are due to residual solvents.

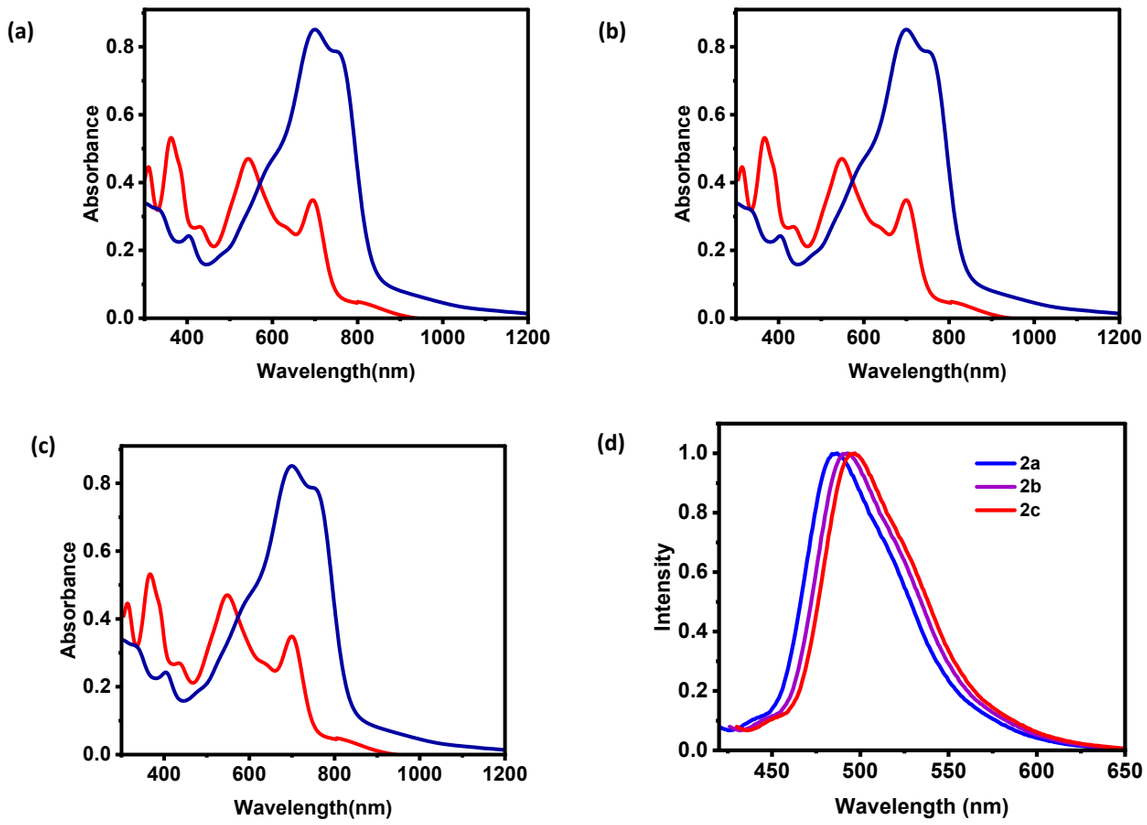


Figure S30. Comparison of absorption spectra of the compounds **2a-c** (10^{-5} M) free base and in presence of TFA (excess) recorded in toluene at room temperature**. (d)** Comparison of normalized emission spectra of compounds **2a-c** recorded in toluene.

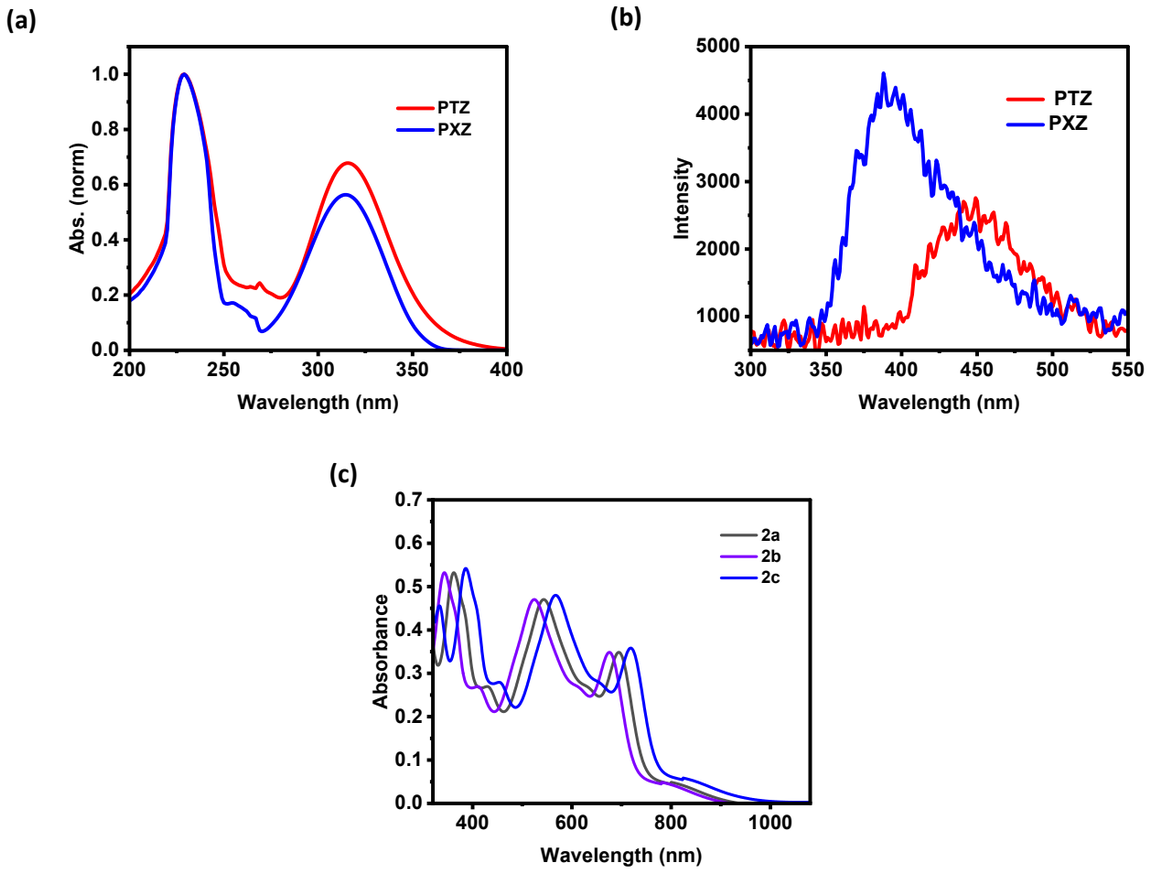


Figure S31. Comparison of absorption and fluorescence spectra of the phenothiazine and phenoxazine unit recorded in acetonitrile at room temperature**.** (c) Comparison of absorption spectra of compound **2a-c** (10^{-5} M) free base recorded in toluene.

Figure S32. Differential pulse voltammogram (blue dotted line) of compounds **2b-c** (IUPAC convention has been followed for plotting Differential pulse voltammogram), recorded in CH_2Cl_2 containing 0.1 M TBAP as the supporting electrolyte and 10^{-3} M of the analyte at scan rates of 50 mVs^{-1} at 25 °C. Saturated calomel electrode (SCE) was used as the reference electrode, glassy carbon as the working electrode and platinum wire as the auxiliary electrode.

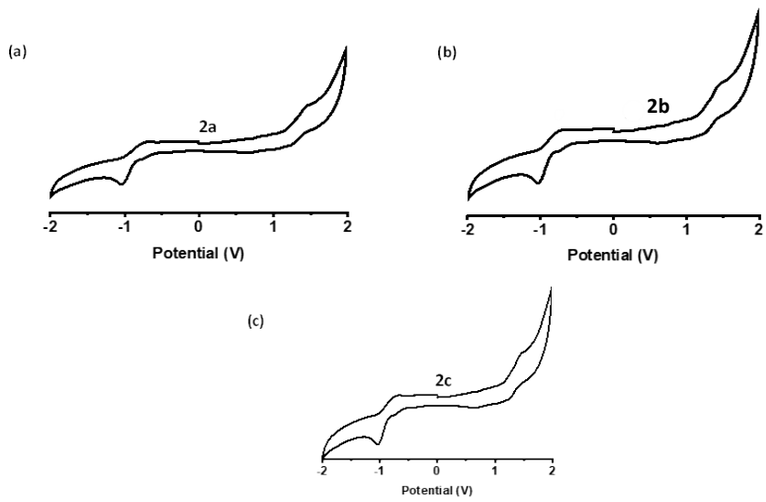


Figure S33. Cyclo voltammogram (black line) of compounds **2a-c** (IUPAC convention has been followed for plotting Cyclic Voltammogram), recorded in CH_2Cl_2 containing 0.1 M TBAP as the supporting electrolyte and 10^{-3} M of the analyte at scan rates of 50 mVs^{-1} at 25 °C. Saturated calomel electrode (SCE) was used as the reference electrode, glassy carbon as the working electrode and platinum wire as the auxiliary electrode.

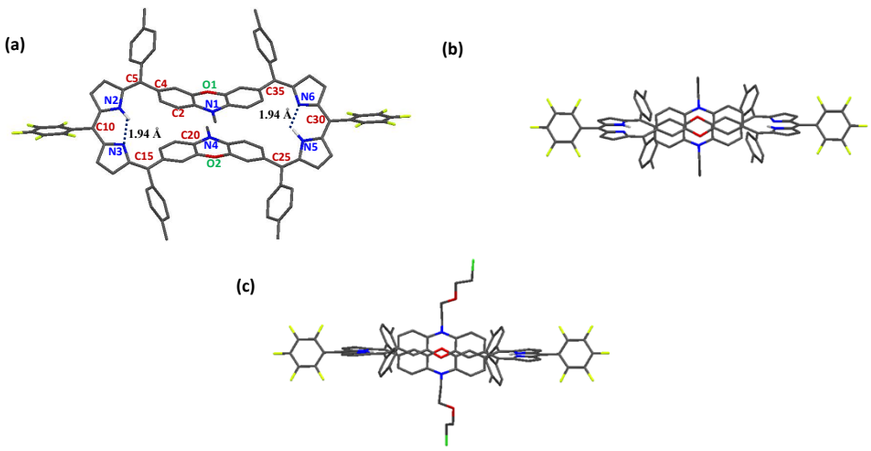


Figure S34. Ground-state optimized structures of phenoxazine embedded hexaphyrins **2a-c** (top view) using B3LYP/6-31g (d,p) level of theory.

Table S1. Calculated HOMO energies, dipole moments, and polarizabilities of phenothiazine embedded hexaphyrin **1a** and phenoxazine embedded hexaphyrin **2a.**

Compound no.	**E_{HOMO}(eV)**	**$E_{HOMO-LUMO}$ (eV)**	**Dipole Moment (debye)**	**Polarizability (a.u.)**
1a	4.41	1.63	3.38	2028.68
2a	4.29	1.71	0.08	1998.32

Table S2. Crystal data and structure refinement for mr_knt_27ma (2b).

Identification code	mr_knt_27_0m_a
Empirical formula	$C_{90}H_{60}F_{10}N_6O_2$
Formula weight	1447.44
Temperature/K	150.00
Crystal system	triclinic
Space group	P-1
a/Å	12.130(11)
b/Å	13.625(12)
c/Å	16.090(15)
α/°	69.226(13)
β/°	86.778(14)
γ/°	82.048(12)
Volume/Å^3	2462(4)
Z	1
ρ_{calc}g/cm^3	0.976
μ/mm^{-1}	0.072
F(000)	748.0
Crystal size/mm^3	0.5 × 0.3 × 0.1
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.322 to 50
Index ranges	$-14 \leq h \leq 14$, $-16 \leq k \leq 16$, $-19 \leq l \leq 19$
Reflections collected	23261
Independent reflections	8436 [R_{int} = 0.1425, R_{sigma} = 0.1962]
Data/restraints/parameters	8436/0/496
Goodness-of-fit on F^2	0.955
Final R indexes [I>=2σ (I)]	R_1 = 0.1052, wR_2 = 0.2474
Final R indexes [all data]	R_1 = 0.2223, wR_2 = 0.3383
Largest diff. peak/hole / e Å^{-3}	0.25/-0.23

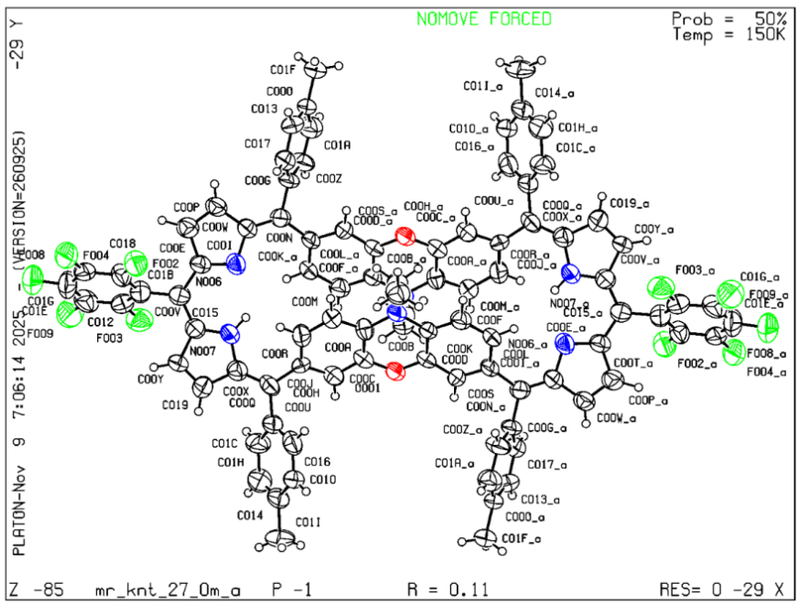


Table S3. Selected TD-DFT calculated oscillator strengths and compositions of the major electronic transitions of **2a**.

No.	Wavelength (nm)	Osc. Strength	Major contribs
1	1041.27146227	0.0	HOMO->LUMO (98%)
2	775.531325528	0.2248	HOMO->L+1 (100%)
3	727.307989747	0.4526	H-1->LUMO (100%)
4	628.850644209	0.0	H-1->L+1 (98%)
5	625.393155169	0.4612	H-2->LUMO (96%)
6	547.029309562	0.0	H-3->LUMO (19%), H-2->L+1 (64%), HOMO->L+3 (10%)
7	541.888955473	0.0	H-3->LUMO (78%), H-2->L+1 (19%)
8	534.875724815	1.1024	HOMO->L+2 (93%)
9	486.040977742	0.0	HOMO->L+3 (83%)
10	481.772655964	0.414	H-3->L+1 (97%)
11	458.013273041	0.0	H-1->L+2 (83%)
12	436.856322935	0.128	H-5->LUMO (11%), H-1->L+3 (81%)
13	414.371822507	0.0	H-2->L+2 (96%)
14	407.012648586	0.9797	H-5->LUMO (79%), H-1->L+3 (12%)
15	394.640459026	0.0	H-4->LUMO (80%)

16	389.65458692	0.0	H-7->L+1 (15%), H-6->LUMO (78%)
17	388.82363663	0.0729	H-7->LUMO (69%), H-6->L+1 (15%)
18	386.846156044	0.0791	H-2->L+3 (92%)
19	381.712979934	0.0016	H-4->L+1 (13%), H-3->L+2 (73%)
20	377.103817179	0.0	H-5->L+1 (74%), HOMO->L+5 (14%)
21	374.280604396	0.0001	H-8->LUMO (31%), HOMO->L+5 (38%), HOMO->L+6 (13%)
22	373.33391452	0.1351	HOMO->L+4 (74%)
23	372.313723348	0.0006	H-8->LUMO (35%), HOMO->L+5 (21%), HOMO->L+6 (14%), HOMO->L+8 (14%)
24	368.846888238	0.3573	H-4->L+1 (45%), H-3->L+2 (14%), HOMO->L+7 (23%)
25	362.601096751	0.0001	H-8->LUMO (14%), HOMO->L+6 (14%), HOMO->L+8 (55%)
26	362.452693929	0.0115	H-9->LUMO (69%), HOMO->L+9 (10%)
27	361.280357283	0.0	H-3->L+3 (19%), HOMO->L+5 (11%), HOMO->L+6 (31%), HOMO->L+8 (16%)
28	356.450544842	0.213	H-4->L+1 (12%), HOMO->L+7 (40%), HOMO->L+9 (10%)
29	356.327613198	0.03	H-3->L+3 (62%)
30	353.442780616	0.0267	HOMO->L+7 (13%), HOMO->L+9 (56%)
31	352.799115079	0.0001	HOMO->L+10 (78%)
32	349.951150222	0.0492	H-8->L+1 (19%), H-6->L+1 (24%), HOMO->L+13 (22%)
33	346.015274091	0.0311	H-10->LUMO (44%), HOMO->L+13 (24%)
34	344.228421934	0.0203	H-10->LUMO (12%), H-6->L+1 (28%), HOMO->L+13 (25%)
35	343.075882045	0.0	H-11->LUMO (33%), HOMO->L+12 (14%)
36	342.365364258	0.0022	HOMO->L+11 (68%)
37	342.308649951	0.0006	HOMO->L+12 (64%)
38	340.195343702	0.0003	H-15->LUMO (19%), H-9->L+1 (34%), HOMO->L+15 (14%)
39	338.837946523	0.0034	H-7->L+1 (55%), H-6->LUMO (10%)
40	338.652844807	0.0476	H-8->L+1 (20%), H-6->L+1 (15%), H-1->L+5 (14%)
41	336.520351253	0.0001	H-20->LUMO (15%), H-11->LUMO (29%)
42	334.549900195	0.099	H-21->LUMO (23%), H-14->LUMO (18%)

43	333.559841303	0.6587	H-10->LUMO (13%), H-8->L+1 (18%), H-1->L+5 (31%)
44	330.756817426	0.0001	H-15->LUMO (12%), H-9->L+1 (14%), H-1->L+4 (39%)
45	328.940340158	0.0405	H-21->LUMO (10%), H-14->LUMO (32%), H-12->LUMO (13%)
46	328.443648871	0.0002	H-13->LUMO (54%), H-12->LUMO (28%), H-12->L+1 (14%)
47	328.40884966	0.003	H-14->LUMO (16%), H-13->LUMO (25%), H-13->L+1 (14%), H-12->LUMO (40%)
48	327.870403311	0.0122	H-1->L+5 (16%), HOMO->L+14 (37%)
49	326.781563512	0.0001	H-17->LUMO (11%), H-1->L+4 (18%), HOMO->L+15 (35%)
50	325.511809216	0.0	H-19->LUMO (19%), H-15->LUMO (37%), H-9->L+1 (22%)

Table S4. Selected TD-DFT calculated oscillator strengths and compositions of the major electronic transitions of **2b**.

No.	Wavelength (nm)	Osc. Strength	Major contribs
1	1012.86000337	0.0	HOMO->LUMO (98%)
2	757.895916696	0.1789	HOMO->L+1 (97%)
3	689.145645113	0.6424	H-1->LUMO (97%)
4	635.490481867	0.5042	H-2->LUMO (97%)
5	610.158430178	0.0	H-1->L+1 (97%)
6	554.391848561	0.0	H-2->L+1 (88%)
7	532.280912773	0.0	H-3->LUMO (96%)
8	531.43674673	1.0814	HOMO->L+2 (94%)
9	478.444829097	0.0	HOMO->L+3 (87%)
10	475.764363055	0.4	H-3->L+1 (97%)
11	451.032023763	0.0	H-1->L+2 (84%)
12	425.390081014	0.0673	H-5->LUMO (16%), H-1->L+3 (76%)
13	421.958932077	0.0	H-2->L+2 (96%)
14	399.949009717	0.8676	H-5->LUMO (74%), H-1->L+3 (15%)
15	390.194155821	0.0	H-4->LUMO (78%)

16	388.82363663	0.1506	H-2->L+3 (93%)
17	386.70136926	0.0	H-7->L+1 (16%), H-6->LUMO (78%)
18	385.139764576	0.0502	H-7->LUMO (66%), H-6->L+1 (15%)
19	378.866899961	0.005	H-4->L+1 (14%), H-3->L+2 (69%)
20	374.043482102	0.0	H-5->L+1 (53%), HOMO->L+5 (31%)
21	373.72778602	0.0652	H-1->L+5 (10%), HOMO->L+4 (76%)
22	369.914350963	0.0	H-8->LUMO (11%), HOMO->L+6 (68%)
23	368.627558459	0.0	H-8->LUMO (48%), HOMO->L+5 (13%)
24	366.091454845	0.2482	H-4->L+1 (34%), H-3->L+2 (12%), HOMO->L+7 (40%)
25	365.950982917	0.0	H-8->LUMO (10%), H-5->L+1 (20%), HOMO->L+5 (34%), HOMO->L+6 (15%)
26	359.896060993	0.0045	H-9->LUMO (70%)
27	357.632955499	0.3528	H-4->L+1 (34%), HOMO->L+7 (43%)
28	356.758245367	0.0	H-8->LUMO (16%), HOMO->L+8 (74%)
29	351.080824047	0.0547	HOMO->L+9 (60%)
30	350.822537597	0.0	H-3->L+3 (89%)
31	347.041910688	0.0919	H-8->L+1 (12%), H-6->L+1 (21%), HOMO->L+9 (17%), HOMO->L+13 (22%)
32	345.706538624	0.0	HOMO->L+12 (74%)
33	344.123325688	0.0473	H-10->LUMO (57%)
34	342.943028275	0.0257	H-6->L+1 (27%), HOMO->L+13 (48%)
35	341.968758308	0.0	H-20->LUMO (13%), H-11->LUMO (27%), HOMO->L+11 (14%)
36	341.065671799	0.0057	H-1->L+11 (13%), HOMO->L+10 (75%)
37	341.056289748	0.0	H-1->L+10 (10%), HOMO->L+11 (70%)
38	338.625096991	0.0	H-12->LUMO (27%), H-9->L+1 (30%), HOMO->L+14 (14%)
39	336.895258443	0.0	H-7->L+1 (52%), H-6->LUMO (11%)
40	335.727573821	0.0041	H-8->L+1 (27%), H-7->LUMO (11%), H-6->L+1 (19%), HOMO->L+15 (10%)
41	335.029029676	0.0	H-11->LUMO (38%), H-7->L+1 (18%)
42	333.973152172	0.0054	H-21->LUMO (24%), H-10->LUMO (14%)

43	329.692583663	0.632	H-8->L+1 (11%), H-1->L+5 (10%), H-1->L+6 (31%), HOMO->L+15 (29%)
44	328.844370507	0.0	H-1->L+4 (39%), HOMO->L+14 (18%)
45	326.988403651	0.0038	H-15->LUMO (39%), H-13->LUMO (18%), H-8->L+1 (20%)
46	326.222683293	0.0	H-14->LUMO (76%), H-13->L+1 (14%)
47	326.196934969	0.0023	H-15->LUMO (25%), H-14->L+1 (16%), H-13->LUMO (56%)
48	325.97395297	0.0	H-16->LUMO (52%)
49	325.34951457	0.0	H-18->LUMO (18%), H-12->LUMO (25%), H-9->L+1 (13%), H-1->L+4 (15%)
50	324.880625245	0.0312	H-1->L+5 (63%), HOMO->L+4 (10%), HOMO->L+15 (12%)

Table S5. Selected TD-DFT calculated oscillator strengths and compositions of the major electronic transitions of **2c**.

No.	**Wavelength (nm)**	**Osc. Strength**	**Major contribs**
1	1001.24519916	0.0001	HOMO->LUMO (98%)
2	753.886616881	0.1774	HOMO->L+1 (97%)
3	688.495074479	0.6535	H-1->LUMO (97%)
4	630.802304819	0.4893	H-2->LUMO (97%)
5	610.188459138	0.0018	H-1->L+1 (97%)
6	551.653806506	0.0002	H-2->L+1 (88%)
7	529.960218048	0.3347	H-3->LUMO (64%), HOMO->L+2 (31%)
8	528.897675165	0.728	H-3->LUMO (32%), HOMO->L+2 (62%)
9	476.752261064	0.0148	HOMO->L+3 (84%)
10	473.655994087	0.3743	H-3->L+1 (94%)
11	451.081252318	0.0053	H-1->L+2 (84%)
12	424.836187679	0.0596	H-5->LUMO (12%), H-1->L+3 (75%)
13	419.957975179	0.0007	H-2->L+2 (96%)
14	400.517486149	0.8368	H-5->LUMO (49%), H-4->LUMO (25%), H-1->L+3 (15%)

15	390.304706328	0.0292	H-5->LUMO (24%), H-4->LUMO (53%)
16	387.402177891	0.0062	H-7->L+1 (10%), H-6->LUMO (70%)
17	386.918590102	0.1525	H-2->L+3 (84%)
18	385.343257225	0.0329	H-7->LUMO (59%), H-6->L+1 (11%), H-2->L+3 (10%)
19	377.908415668	0.0199	H-4->L+1 (20%), H-3->L+2 (65%)
20	374.032198058	0.0293	H-5->L+1 (42%), H-4->L+1 (18%), HOMO->L+5 (21%)
21	371.945140134	0.0792	HOMO->L+4 (60%), HOMO->L+5 (11%)
22	370.13521513	0.0003	H-8->LUMO (38%), HOMO->L+6 (31%), HOMO->L+8 (10%)
23	368.507038229	0.0005	H-8->LUMO (24%), HOMO->L+5 (14%), HOMO->L+6 (39%)
24	365.799825964	0.2234	H-4->L+1 (24%), H-3->L+2 (13%), HOMO->L+5 (11%), HOMO->L+7 (27%)
25	364.766675529	0.0192	H-5->L+1 (16%), HOMO->L+4 (13%), HOMO->L+5 (24%), HOMO->L+6 (17%)
26	360.38773657	0.002	H-9->LUMO (64%)
27	357.334043324	0.1692	HOMO->L+7 (22%), HOMO->L+8 (42%)
28	356.419803979	0.1472	H-4->L+1 (11%), HOMO->L+7 (29%), HOMO->L+8 (35%)
29	350.663780898	0.0546	H-8->L+1 (10%), H-6->L+1 (12%), HOMO->L+9 (43%), HOMO->L+11 (10%)
30	349.438271222	0.0044	H-3->L+3 (81%)
31	348.055114851	0.0606	H-6->L+1 (16%), HOMO->L+9 (36%)
32	344.956299071	0.0044	H-6->L+1 (12%), HOMO->L+11 (34%), HOMO->L+12 (14%)
33	344.620710488	0.0426	H-10->LUMO (55%)
34	342.450470963	0.0084	H-20->LUMO (12%), H-11->LUMO (28%)
35	341.469588841	0.0313	HOMO->L+13 (48%)
36	339.394467746	0.0011	HOMO->L+11 (23%), HOMO->L+12 (52%)
37	339.051063805	0.0023	H-1->L+10 (11%), HOMO->L+10 (62%)
38	338.625096991	0.0066	H-12->LUMO (13%), H-8->L+1 (10%), H-7->L+1

			(12%), HOMO->L+10 (15%), HOMO->L+13 (13%)
39	338.264788727	0.0034	H-9->L+1 (21%), H-7->L+1 (12%), HOMO->L+12 (11%)
40	336.027842405	0.0023	H-20->LUMO (13%), H-11->LUMO (28%)
41	334.477697778	0.0044	H-21->LUMO (24%), H-7->L+1 (10%)
42	334.153172198	0.009	H-14->LUMO (14%), H-8->L+1 (11%), H-7->L+1 (31%)
43	329.604936762	0.5629	H-8->L+1 (10%), H-1->L+4 (12%), H-1->L+6 (33%), HOMO->L+15 (13%)
44	328.556797255	0.0646	H-1->L+4 (29%), HOMO->L+15 (13%)
45	327.87907392	0.0018	H-16->LUMO (10%), H-14->LUMO (45%), H-8->L+1 (18%)
46	327.714410732	0.0014	H-15->LUMO (84%), H-15->L+1 (13%)
47	327.290515317	0.0022	H-13->LUMO (78%), H-13->L+1 (19%)
48	326.583587115	0.0003	H-16->LUMO (36%), H-14->LUMO (11%), H-12->LUMO (12%), H-9->L+1 (14%)
49	325.982523564	0.0072	H-18->LUMO (31%), H-12->LUMO (11%), H-1->L+4 (12%)
50	324.82955543	0.0188	H-17->LUMO (27%), H-1->L+4 (10%), HOMO->L+14 (14%)

Table S6. S_0 optimized geometry of compound **2a** at B3LYP/6-31g (d,p) level of theory

Sum of imaginary frequencies= 0

Total Energy (Hartree) = -4864.415290

Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-3.424177000	-1.212954000	1.015881000	C	-3.257601000	-2.229975000	-0.057299000
C	-1.938590000	-2.473177000	0.392754000	C	-0.871776000	-1.757043000	-0.105432000
C	-1.033041000	-0.751275000	-1.077647000	C	-2.339675000	-0.495128000	-1.517399000
O	-0.383541000	-2.038908000	0.408704000	C	1.442051000	-1.768332000	-0.438701000
C	1.336566000	-0.752942000	-1.406588000	N	0.107292000	-0.077898000	-1.534251000
C	2.591335000	-2.520377000	-0.288102000	C	3.702085000	-2.296639000	-1.119656000
C	3.628658000	-1.253078000	-2.047424000	C	2.462930000	-0.491846000	-2.193510000

C	-0.014151000	0.973590000	-2.531156000	C	-4.352720000	-3.088714000	0.411759000
C	4.886150000	-3.201121000	-1.066470000	C	4.758060000	-4.562065000	-1.626716000
C	6.079008000	-2.734905000	-0.578637000	C	-4.015190000	-4.468078000	0.838323000
C	-5.679136000	-2.706805000	0.446315000	C	-6.839665000	-3.563941000	0.606009000
C	-7.963207000	-2.802430000	0.516650000	N	-6.189128000	-1.425522000	0.267290000
N	6.334327000	-1.413508000	-0.223079000	C	8.230192000	-2.577002000	0.177976000
C	7.307805000	-3.458421000	-0.282812000	C	5.814637000	-5.146767000	-2.358261000
C	5.705711000	-6.426809000	-2.894402000	C	4.532041000	-7.177168000	-2.749861000
C	3.466348000	-6.589099000	-2.055419000	C	3.568037000	-5.310104000	-1.515878000
C	-3.168635000	-5.277545000	0.055685000	C	-2.861409000	-6.576845000	0.444088000
C	-3.373260000	-7.119307000	1.633555000	C	-4.206823000	-6.313861000	2.418041000
C	-4.519522000	-5.010204000	2.032803000	C	4.402185000	-8.549375000	-3.362711000
C	-3.008332000	-8.519139000	2.062050000	C	7.634240000	-1.254057000	0.183225000
C	-7.561093000	-1.428313000	0.312651000	C	-7.771997000	1.017483000	0.051855000
C	7.498101000	1.202706000	0.411973000	C	-4.508248000	8.747093000	-1.825367000
C	3.999483000	8.745173000	-1.444108000	C	-5.525892000	5.068602000	-1.683858000
C	-5.409208000	6.394145000	-2.098422000	C	-4.660283000	7.319737000	-1.361192000
C	-4.027760000	6.874226000	-0.190151000	C	-4.137168000	5.552239000	0.226946000
C	5.120956000	5.095228000	-1.417007000	C	4.991222000	6.436899000	-1.771759000
C	4.163789000	7.300188000	-1.043031000	C	3.467908000	6.776620000	0.057605000
C	3.587801000	5.437246000	0.412423000	C	7.092370000	3.411015000	0.224709000
C	8.104893000	2.529697000	0.426470000	N	6.170777000	1.272827000	0.248340000
N	-6.451370000	1.234432000	0.101125000	C	-8.499360000	2.261668000	-0.190474000
C	-7.561432000	3.237295000	-0.296415000	C	-6.263727000	2.593388000	-0.099205000
C	-4.901715000	4.621761000	-0.504955000	C	5.865210000	2.622187000	0.140082000
C	4.426465000	4.568897000	-0.313211000	C	4.583207000	3.147985000	0.075429000
C	-5.030188000	3.222067000	-0.047715000	C	-0.309912000	-0.400538000	2.789075000
C	2.210219000	0.759083000	1.816445000	C	3.390996000	1.342255000	1.365063000
C	3.378682000	2.398410000	0.434653000	C	2.115670000	2.806063000	-0.053484000
N	-0.262162000	0.658458000	1.790666000	C	0.955356000	1.186177000	1.353135000
C	0.951271000	2.222345000	0.394365000	O	-0.220985000	2.707186000	-0.146171000
C	-2.707358000	0.958571000	1.929069000	C	-1.449083000	1.285067000	1.400932000
C	-1.409614000	2.293099000	0.416451000	C	-2.555449000	2.904701000	-0.046335000

C	-3.827298000	2.547831000	0.454014000	C	-3.867776000	1.569419000	1.462610000
C	-8.350595000	-0.286754000	0.193488000	C	8.224564000	-0.035061000	0.484298000
C	-9.822507000	-0.427380000	0.218699000	C	-10.511605000	-1.249525000	-0.684013000
C	-11.897391000	-1.383968000	-0.664921000	C	-12.647045000	-0.665786000	0.263099000
C	-11.999782000	0.169861000	1.170282000	C	-10.611656000	0.269144000	1.145555000
F	-9.834291000	-1.944233000	-1.613323000	F	-12.515798000	-2.181041000	-1.547543000
F	-13.980047000	-0.779537000	0.284819000	F	-12.715288000	0.852535000	2.074958000
F	-10.028597000	1.063639000	2.057316000	F	10.334479000	-1.076585000	-1.173196000
F	12.934876000	-0.985580000	-0.483773000	F	13.700592000	0.185232000	1.863061000
F	11.815926000	1.249437000	3.530839000	F	9.201739000	1.123516000	2.880494000
C	10.660638000	-0.515427000	0.003253000	C	12.011155000	-0.472414000	0.340906000
C	12.405429000	0.130485000	1.532436000	C	11.442567000	0.676027000	2.378683000
C	10.097734000	0.601051000	2.028891000	C	9.660985000	0.005334000	0.836445000
H	-4.406934000	-1.004067000	-1.420339000	H	-1.736741000	-3.244126000	1.126336000
H	-2.519222000	0.253988000	-2.277457000	H	2.608038000	-3.288486000	0.476818000
H	4.476656000	-1.054030000	-2.694568000	H	2.431296000	0.284430000	-2.947618000
H	-0.901650000	1.567982000	-2.320450000	H	0.848582000	1.637003000	-2.445762000
H	-0.068114000	0.569456000	-3.552276000	H	-6.782334000	-4.635097000	0.726975000
H	-8.988265000	-3.137021000	0.573183000	H	-5.701371000	-0.526414000	0.222126000
H	5.712233000	-0.606711000	-0.281871000	H	9.236893000	-2.791756000	0.505232000
H	7.419334000	-4.526753000	-0.386967000	H	6.716821000	-4.572385000	-2.535375000
H	6.539720000	-6.843636000	-3.453767000	H	2.539139000	-7.144399000	-1.935964000
H	2.714601000	-4.892535000	-0.996865000	H	-2.763885000	-4.876620000	-0.868105000
H	-2.219041000	-7.187238000	-0.186005000	H	-4.607692000	-6.709423000	3.347899000
H	-5.153103000	-4.394415000	2.663101000	H	3.721193000	-9.179985000	-2.781249000
H	4.001124000	-8.488628000	-4.383461000	H	5.374212000	-9.050263000	-3.422216000
H	-3.706473000	-8.898376000	2.815016000	H	-2.000830000	-8.546946000	2.497982000
H	-3.010758000	-9.206920000	1.209002000	H	-4.537672000	9.443164000	-0.979789000
H	-3.546134000	8.894238000	-2.334026000	H	-5.300473000	9.021732000	-2.529082000
H	3.893667000	9.390057000	-0.564940000	H	3.099487000	8.881853000	-2.058510000
H	4.855676000	9.093732000	-2.030509000	H	-6.092271000	4.359792000	-2.278370000
H	-5.898099000	6.714972000	-3.014822000	H	-3.447209000	7.577651000	0.401605000
H	-3.643472000	5.227174000	1.136949000	H	5.757967000	4.435665000	-1.996846000

H	5.535393000	6.820593000	-2.631054000	H	2.829543000	7.432501000	0.644286000
H	3.044529000	5.051525000	1.268811000	H	7.143829000	4.489875000	0.199145000
H	9.156971000	2.742412000	0.558682000	H	-9.573312000	2.363263000	-0.265788000
H	-7.719011000	4.296166000	-0.442262000	H	0.571083000	-1.030398000	2.698044000
H	-0.382610000	0.004490000	3.806957000	H	-1.170782000	-1.039464000	2.585647000
H	2.276034000	-0.016464000	2.567974000	H	4.337225000	1.003225000	1.764688000
H	2.033244000	3.610736000	-0.774053000	H	-2.788926000	0.227428000	2.722356000
H	-2.454185000	3.668129000	-0.808655000	H	-4.820797000	1.292960000	1.892585000

Table S7. S_0 optimized geometry of compound **2b** at B3LYP/6-31g (d,p) level of theory

Sum of imaginary frequencies= 0

Total Energy (Hartree) = -4943.072265

Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
O	-2.373639000	-0.657629000	-1.029825000	F	-0.312495000	9.860706000	-3.036706000
F	-0.259502000	7.368239000	-7.075649000	F	-0.306312000	12.149765000	-4.460033000
N	-1.307903000	0.658230000	1.216631000	N	1.021209000	5.788873000	-2.740114000
N	-1.541598000	5.249866000	-3.603727000	H	-0.768550000	4.893263000	-3.041772000
F	-0.297685000	12.071461000	-7.190748000	F	-0.282213000	9.664563000	-8.482869000
C	-1.756861000	1.399407000	0.113885000	C	-1.637926000	-0.700363000	1.290310000
C	-2.307871000	0.721073000	-0.993341000	C	-2.194092000	-1.336821000	0.161198000
C	0.881991000	6.936030000	-3.425964000	C	-1.445290000	-1.495778000	2.433081000
H	-1.043145000	-1.057935000	3.337579000	C	4.020367000	5.186134000	-0.503604000
C	-2.775485000	1.392149000	-2.104519000	H	-3.193749000	0.804010000	-2.913019000
C	2.254709000	5.866116000	-2.097585000	C	-2.705915000	2.800071000	-2.194781000
C	-2.361687000	-3.470007000	1.322817000	C	-1.785756000	-2.846672000	2.444698000
H	-1.631356000	-3.421592000	3.348648000	C	-1.689622000	2.798828000	0.027886000
H	-1.299507000	3.377210000	0.855271000	C	2.833392000	4.860612000	-1.335782000
C	6.305008000	5.815155000	1.073338000	C	2.051847000	7.796719000	-3.260545000
H	2.211999000	8.755814000	-3.732973000	C	-3.283741000	3.488039000	-3.361640000
C	-2.143264000	3.480473000	-1.101364000	H	-2.097472000	4.563681000	-1.101759000
C	-2.555641000	-2.667587000	0.175279000	H	-2.985038000	-3.083574000	-0.728424000
C	-0.296043000	9.778539000	-4.377380000	C	-4.497436000	2.895127000	-3.979281000
C	-1.391114000	6.432689000	-4.286754000	C	2.889604000	7.144105000	-2.417368000

H	3.868774000	7.460164000	-2.088666000	C	-2.771807000	4.655514000	-3.892274000
C	-2.610576000	6.626558000	-5.043236000	H	-2.823497000	7.490682000	-5.655154000
C	5.174706000	4.378349000	-0.535912000	H	5.195535000	3.506101000	-1.181625000
C	-6.727169000	1.935563000	-3.753214000	H	-7.553020000	1.638593000	-3.111457000
C	-0.682638000	1.334276000	2.358342000	H	-0.067939000	2.145929000	1.964549000
H	0.018266000	0.632782000	2.814431000	C	-0.282510000	8.523639000	-4.999085000
C	5.152023000	6.608080000	1.122363000	H	5.124813000	7.472016000	1.781401000
C	-6.840352000	1.770916000	-5.143579000	C	-0.272317000	7.258141000	-4.215644000
C	-5.581483000	2.476715000	-3.181259000	H	-5.525906000	2.597623000	-2.103901000
C	4.031609000	6.303942000	0.349588000	H	3.143998000	6.923984000	0.422073000
C	-0.292261000	10.969832000	-5.096431000	C	-3.424489000	5.561059000	-4.820484000
H	-4.419918000	5.412590000	-5.210306000	C	6.292404000	4.693061000	0.229048000
H	7.173043000	4.058183000	0.171551000	C	-0.276117000	8.529029000	-6.399488000
C	-4.608869000	2.720329000	-5.369919000	H	-3.777084000	2.999361000	-6.008964000
C	-1.681536000	1.859224000	3.394411000	H	-2.368239000	2.585916000	2.951415000
H	-1.144591000	2.350993000	4.211381000	H	-2.277394000	1.046176000	3.818470000
C	-0.292430000	10.933139000	-6.487644000	C	7.528639000	6.157364000	1.888012000
H	8.298000000	6.628256000	1.263694000	H	7.978161000	5.262186000	2.329309000
H	7.289364000	6.853964000	2.695915000	C	-0.288500000	9.705878000	-7.142795000
C	-5.759622000	2.172570000	-5.937269000	H	-5.812109000	2.046221000	-7.015584000
C	-8.078583000	1.158296000	-5.751722000	H	-8.126873000	0.081216000	-5.550481000
H	-8.100123000	1.293397000	-6.836283000	H	-8.988550000	1.602031000	-5.334444000
O	2.373639000	0.657629000	1.029825000	F	0.312495000	-9.860706000	3.036706000
F	0.259502000	-7.368239000	7.075649000	F	0.306312000	-12.149765000	4.460033000
N	1.307903000	-0.658230000	-1.216631000	N	-1.021209000	-5.788873000	2.740114000
N	1.541598000	-5.249866000	3.603727000	H	0.768550000	-4.893263000	3.041772000
F	0.297685000	-12.071461000	7.190748000	F	0.282213000	-9.664563000	8.482869000
C	1.756861000	-1.399407000	-0.113885000	C	1.637926000	0.700363000	-1.290310000
C	2.307871000	-0.721073000	0.993341000	C	2.194092000	1.336821000	-0.161198000
C	-0.881991000	-6.936030000	3.425964000	C	1.445290000	1.495778000	-2.433081000
H	1.043145000	1.057935000	-3.337579000	C	-4.020367000	-5.186134000	0.503604000
C	2.775485000	-1.392149000	2.104519000	H	3.193749000	-0.804010000	2.913019000
C	-2.254709000	-5.866116000	2.097585000	C	2.705915000	-2.800071000	2.194781000

C	2.361687000	3.470007000	-1.322817000	C	1.785756000	2.846672000	-2.444698000
H	1.631356000	3.421592000	-3.348648000	C	1.689622000	-2.798828000	-0.027886000
H	1.299507000	-3.377210000	-0.855271000	C	-2.833392000	-4.860612000	1.335782000
C	-6.305008000	-5.815155000	-1.073338000	C	-2.051847000	-7.796719000	3.260545000
H	-2.211999000	-8.755814000	3.732973000	C	3.283741000	-3.488039000	3.361640000
C	2.143264000	-3.480473000	1.101364000	H	2.097472000	-4.563681000	1.101759000
C	2.555641000	2.667587000	-0.175279000	H	2.985038000	3.083574000	0.728424000
C	0.296043000	-9.778539000	4.377380000	C	4.497436000	-2.895127000	3.979281000
C	1.391114000	-6.432689000	4.286754000	C	-2.889604000	-7.144105000	2.417368000
H	-3.868774000	-7.460164000	2.088666000	C	2.771807000	-4.655514000	3.892274000
C	2.610576000	-6.626558000	5.043236000	H	2.823497000	-7.490682000	5.655154000
C	-5.174706000	-4.378349000	0.535912000	H	-5.195535000	-3.506101000	1.181625000
C	6.727169000	-1.935563000	3.753214000	H	7.553020000	-1.638593000	3.111457000
C	0.682638000	-1.334276000	-2.358342000	H	0.067939000	-2.145929000	-1.964549000
H	-0.018266000	-0.632782000	-2.814431000	C	0.282510000	-8.523639000	4.999085000
C	-5.152023000	-6.608080000	-1.122363000	H	-5.124813000	-7.472016000	-1.781401000
C	6.840352000	-1.770916000	5.143579000	C	0.272317000	-7.258141000	4.215644000
C	5.581483000	-2.476715000	3.181259000	H	5.525906000	-2.597623000	2.103901000
C	-4.031609000	-6.303942000	-0.349588000	H	-3.143998000	-6.923984000	-0.422073000
C	0.292261000	-10.969832000	5.096431000	C	3.424489000	-5.561059000	4.820484000
H	4.419918000	-5.412590000	5.210306000	C	-6.292404000	-4.693061000	-0.229048000
H	-7.173043000	-4.058183000	-0.171551000	C	0.276117000	-8.529029000	6.399488000
C	4.608869000	-2.720329000	5.369919000	H	3.777084000	-2.999361000	6.008964000
C	1.681536000	-1.859224000	-3.394411000	H	2.368239000	-2.585916000	-2.951415000
H	1.144591000	-2.350993000	-4.211381000	H	2.277394000	-1.046176000	-3.818470000
C	0.292430000	-10.933139000	6.487644000	C	-7.528639000	-6.157364000	-1.888012000
H	-8.298000000	-6.628256000	-1.263694000	H	-7.978161000	-5.262186000	-2.329309000
H	-7.289364000	-6.853964000	-2.695915000	C	0.288500000	-9.705878000	7.142795000
C	5.759622000	-2.172570000	5.937269000	H	5.812109000	-2.046221000	7.015584000
C	8.078583000	-1.158296000	5.751722000	H	8.126873000	-0.081216000	5.550481000
H	8.100123000	-1.293397000	6.836283000	H	8.988550000	-1.602031000	5.334444000

Table S8. S_0 optimized geometry of compound **2c** at B3LYP/6-31g (d,p) level of theory

Sum of imaginary frequencies= 0

Total Energy (Hartree) = -6169.932452.

Atom	X	Y	Z	Atom	X	Y	Z
O	0.153736000	-2.745579000	0.095561000	F	10.169925000	0.934681000	-2.234247000
F	10.081190000	-0.989319000	2.103620000	F	12.863477000	0.980688000	-2.148774000
N	0.084668000	-0.709355000	-1.854266000	N	6.482215000	1.307407000	-0.054984000
N	6.524170000	-1.448315000	-0.205791000	H	5.910618000	-0.634634000	-0.162123000
F	14.186632000	0.029702000	0.043722000	F	12.773850000	-0.960300000	2.162243000
C	1.304634000	-1.298806000	-1.487710000	C	-1.108987000	-1.288048000	-1.395535000
C	1.311536000	-2.337738000	-0.533524000	C	-1.050564000	-2.311697000	-0.428140000
C	7.821815000	1.208696000	-0.097696000	C	-2.388133000	-0.908682000	-1.836004000
H	-2.486562000	-0.176996000	-2.625776000	C	4.753100000	4.671177000	-0.294725000
C	2.475105000	-2.974510000	-0.152952000	H	2.399605000	-3.771424000	0.577607000
C	6.191351000	2.669303000	-0.082851000	C	3.727665000	-2.599678000	-0.687192000
C	-3.474359000	-2.538756000	-0.373258000	C	-3.538462000	-1.508788000	-1.330277000
H	-4.503743000	-1.197885000	-1.708423000	C	2.550094000	-0.917210000	-2.011441000
H	2.612825000	-0.134749000	-2.756135000	C	4.925285000	3.228544000	0.017354000
C	4.439876000	7.439757000	-0.875526000	C	8.449249000	2.528544000	-0.134070000
H	9.510963000	2.731999000	-0.133659000	C	4.933968000	-3.361630000	-0.323168000
C	3.731608000	-1.545353000	-1.615991000	H	4.660101000	-1.234305000	-2.081316000
C	-2.186404000	-2.923793000	0.061281000	H	-2.058244000	-3.706872000	0.799043000
C	10.781532000	0.467724000	-1.133198000	C	4.777279000	-4.818027000	-0.074836000
C	7.885777000	-1.272166000	-0.142612000	C	7.437990000	3.431344000	-0.150209000
H	7.518228000	4.508434000	-0.145222000	C	6.193489000	-2.804874000	-0.222800000
C	8.470845000	-2.596632000	-0.145757000	H	9.531496000	-2.800167000	-0.146516000
C	4.055456000	5.526780000	0.581988000	H	3.643332000	5.124145000	1.501953000
C	3.910237000	-6.993843000	-0.750726000	H	3.356401000	-7.594083000	-1.468329000
C	0.076083000	0.479725000	-2.706920000	H	0.925221000	1.107196000	-2.424746000
H	-0.818485000	1.061323000	-2.478839000	C	10.018485000	-0.025468000	-0.067464000
C	5.121163000	6.589613000	-1.754072000	H	5.532218000	6.992244000	-2.676167000
C	4.478516000	-7.613849000	0.373926000	C	8.530382000	-0.038959000	-0.105387000
C	4.047429000	-5.627387000	-0.968334000	H	3.602472000	-5.177821000	-1.850566000

C	5.276417000	5.231958000	-1.472708000	H	5.794839000	4.592183000	-2.179456000
C	12.172371000	0.499935000	-1.105474000	C	7.462963000	-3.507751000	-0.176820000
H	7.560621000	-4.581774000	-0.218803000	C	3.913540000	6.880604000	0.300958000
H	3.388928000	7.519084000	1.007438000	C	10.736059000	-0.501214000	1.036978000
C	5.338232000	-5.439261000	1.055089000	H	5.877600000	-4.837367000	1.779634000
C	0.142937000	0.210855000	-4.208915000	H	0.988048000	-0.450762000	-4.448918000
H	0.311911000	1.168444000	-4.726617000	C	12.849355000	0.012082000	0.008284000
C	4.245072000	8.903544000	-1.187852000	H	4.379842000	9.523563000	-0.295889000
H	3.230558000	9.095591000	-1.559159000	H	4.945964000	9.245481000	-1.953603000
C	12.127261000	-0.494964000	1.083910000	C	5.193056000	-6.809743000	1.269977000
H	5.635425000	-7.258682000	2.155584000	C	4.297040000	-9.092252000	0.618178000
H	3.296849000	-9.307284000	1.014180000	H	5.024855000	-9.470487000	1.341015000
H	4.404615000	-9.665562000	-0.308060000	O	0.117483000	2.681084000	-0.119520000
F	-9.906414000	-0.892073000	2.282107000	F	-9.825248000	0.858543000	-2.129085000
F	-12.599758000	-0.943547000	2.202129000	N	0.141877000	0.656182000	1.840891000
N	-6.220610000	-1.346693000	0.111424000	N	-6.263515000	1.407183000	0.152185000
H	-5.651343000	0.591187000	0.141936000	F	-13.926850000	-0.080516000	-0.024214000
F	-12.517706000	0.826378000	-2.182028000	C	-1.069995000	1.262847000	1.464992000
C	1.343895000	1.222267000	1.395791000	C	-1.055309000	2.281695000	0.491030000
C	1.307716000	2.260745000	0.441911000	C	-7.560039000	-1.249159000	0.157797000
C	2.615671000	0.819232000	1.839636000	H	2.711260000	0.033381000	2.577678000
C	-4.482585000	-4.694522000	0.468570000	C	-2.208617000	2.918763000	0.078452000
H	-2.116368000	3.698125000	-0.668867000	C	-5.925370000	-2.705236000	0.193908000
C	-3.469739000	2.565857000	0.605219000	C	3.732842000	2.486837000	0.446690000
C	3.778624000	1.427007000	1.370177000	H	4.736617000	1.095098000	1.749068000
C	-2.320794000	0.916616000	1.997856000	H	-2.380853000	0.191421000	2.797306000
C	-4.658788000	-3.265269000	0.101232000	C	-4.166647000	-7.438242000	1.156057000
C	-8.183438000	-2.567856000	0.254521000	H	-9.244523000	-2.773981000	0.269728000
C	-4.669146000	3.319020000	0.201881000	C	-3.490309000	1.544482000	1.571424000
H	-4.425135000	1.263984000	2.043540000	C	2.454053000	2.882438000	-0.007224000
H	2.343618000	3.679156000	-0.733259000	C	-10.519600000	-0.469705000	1.164058000
C	-4.506565000	4.763743000	-0.102909000	C	-7.625104000	1.230745000	0.096522000
C	-7.169358000	-3.466565000	0.304002000	H	-7.246646000	-4.543082000	0.346548000

C	-5.930071000	2.762490000	0.115834000	C	-8.207780000	2.555350000	0.043975000
H	-9.268060000	2.760713000	0.035406000	C	-3.802390000	-5.587333000	-0.384525000
H	-3.403385000	-5.223277000	-1.326086000	C	-3.639522000	6.963268000	0.491852000
H	-3.089296000	7.590544000	1.188852000	C	0.164010000	-0.535406000	2.690046000
H	-0.753740000	-1.099838000	2.516135000	H	0.983132000	-1.176596000	2.355119000
C	-9.758231000	-0.018520000	0.078550000	C	-4.827552000	-6.550225000	2.012212000
H	-5.219981000	-6.912487000	2.958837000	C	-4.198914000	7.539202000	-0.660415000
C	-8.270244000	-0.002862000	0.113522000	C	-3.781199000	5.606876000	0.762744000
H	-3.343420000	5.191890000	1.665269000	C	-4.985355000	-5.204764000	1.677797000
H	-5.487324000	-4.534369000	2.367868000	C	-11.910459000	-0.503926000	1.139589000
C	-7.198115000	3.465238000	0.038177000	H	-7.293998000	4.540277000	0.035663000
C	-3.658278000	-6.928820000	-0.050652000	H	-3.144765000	-7.596535000	-0.738083000
C	-10.477932000	0.412961000	-1.042651000	C	-5.058499000	5.340764000	-1.260359000
H	-5.594095000	4.711419000	-1.964081000	C	0.328002000	-0.274884000	4.186221000
H	0.532856000	-1.234479000	4.685422000	H	1.187437000	0.384584000	4.365544000
C	-12.589442000	-0.060716000	0.008546000	C	-3.991638000	-8.894555000	1.512205000
H	-4.405601000	-9.545624000	0.734123000	H	-2.931331000	-9.153891000	1.612937000
H	-4.487601000	-9.137864000	2.455212000	C	-11.869193000	0.404189000	-1.087142000
C	-4.908960000	6.701394000	-1.528618000	H	-5.344325000	7.115592000	-2.434414000
C	-4.013646000	9.006730000	-0.961025000	H	-3.003762000	9.208411000	-1.338954000
H	-4.723126000	9.352504000	-1.717518000	H	-4.146803000	9.617629000	-0.062435000
O	-1.075956000	-0.377449000	-4.636522000	O	-0.872431000	0.295479000	4.694869000
C	-0.830636000	0.629083000	6.075752000	H	-1.857495000	0.576798000	6.447859000
H	-0.223497000	-0.090291000	6.640442000	C	-0.288435000	2.045828000	6.258794000
H	0.739267000	2.146486000	5.910174000	H	-0.919650000	2.776386000	5.753771000
C	-1.082747000	-0.700908000	-6.017305000	H	-0.941155000	0.198808000	-6.634096000
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H	-2.584648000	-2.239015000	-5.721959000	H	-3.250455000	-0.629876000	-6.103097000
Cl	-0.278029000	2.487215000	8.026514000	Cl	-2.555222000	-1.790959000	-8.056789000

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