Synthesis of Anthracene Bridged Expanded Rosarin

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General Experimental Section

All the chemicals used for the synthesis were of reagent grade unless otherwise specified. Boron trifluoride diethyl etherate ($BF_3.OEt_2$), trifluoroacetic acid (TFA), and 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ) obtained from Sigma-Aldrich were used as such. All other chemicals used for the synthesis were of reagent grade unless otherwise specified. Solvents such as petroleum ether (60-80°C), ethyl acetate, and dichloromethane purchased from Merck, India, and were used without further purification. Column chromatography was performed on aluminium oxide active basic (70-200 mesh, pH value 8.5-10). ^1H (1D and 2D) and $^{13}C\{^1H\}$ NMR spectra were recorded on a Bruker 400 and 500 MHz FT-NMR spectrometers in $CDCl_3$ using tetramethylsilane as the internal reference. The $^{13}C\{^1H\}$ NMR frequencies are 125.77 and 100.06 MHz for 500 and 400 MHz instruments, respectively. Structural assignments were made with additional information from ^1H-^1H COSY and ^1H -^1H NOESY experiments. The high-resolution mass spectroscopy (HR-MS) were recorded with a Bruker maXis Impact and QT of micro mass spectrometer using positive mode ESI methods in acetonitrile or methanol. Matrix-assisted laser desorption ionization time-of-flight mass spectrometries (MALDI-TOF-MS) were recorded on a Bruker autoflex maX. UV−visible absorption spectra were recorded on a Cary Series UV−Vis−NIR and a UV 3600 Shimadzu spectrophotometer. Steady-state fluorescence spectra were obtained with Horiba FluoroMax 4 instruments. The stock solutions of the compounds (10^{-5} M) were prepared using HPLC-grade Toluene.

Computational details: All the calculations were carried out using Gaussian 09 program package.[1] The density functional theory (DFT)[2] method, hybrid functional B3LYP in conjunction with basis set 6-31G(d,p)[3] assisted in optimizing the structures of the compound **3** in ground (S_0) states. For $S_0 \rightarrow S_n$ transitions the oscillator strengths were derived using identical basis and functional hybrid set whereas the vertical excitation energies were obtained by the help of TD-DFT techniques. Under the Polarisable Continuum Model (PCM)[4] 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 on the basis of the optimized structures in the S_0 state.

X-ray Crystallography. X-ray diffraction data were collected using a Bruker D8 QUEST single-crystal X-ray diffractometer with Mo K_α radiation. The data collection was evaluated by using the Crystal Clear-SM Expert software. The data were collected by a standard ω-scan technique. The structure was solved by a direct method using SHELXT-2018/2 and refined by full matrix least squares with SHELXL-2018/3 refining on F^2.[5] All data were corrected for Lorentz and polarization effects, and all non-hydrogen atoms were refined anisotropically. The remaining hydrogen atoms were placed in geometrically constrained positions and refined with isotropic temperature factors, generally 1.2Ueq of their parent atoms. Hydrogen atoms were included in the refinement process as per the riding model. CCDC 2374821 contained the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Experimental Section:

The starting precursor 1,8-dibromoanthracene is commercially available compound. The compounds **3, 4** and **5** were prepared as described below:

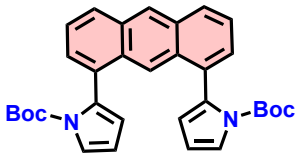
Di-tert-butyl 2,2'-(anthracene-1,8-diyl)bis(1H-pyrrole-1-carboxylate) (4): In round bottom flask, 1,8-dibromoanthracene (0.5 g, 1.48 mmol), (1-(tert-butoxycarbonyl)-1H-pyrrol-2-yl)boronic acid (1.26 g, 5.95 mmol) and tetrakis(triphenylphosphine)-palladium(0) (5 mol%) were dissolved in 1,4-dioxane (50 mL) and K_2CO_3 (4 g, 2 M) was added and the reaction mixture was refluxed for 1 h at 105 ^oC, with vigorous stirring under nitrogen atmosphere. After completion of the reaction, as judged by TLC analysis, the reaction mixture was diluted with water and extracted with dichloromethane. The combined organic layers were washed with

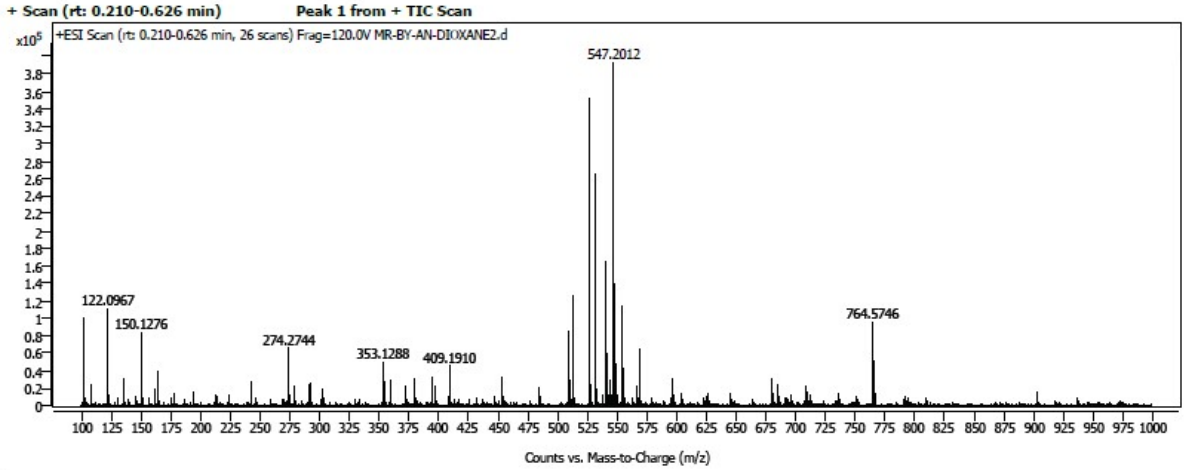
water and dried over sodium sulphate. After evaporation, the crude product was purified by silica chromatography using a petroleum ether to afford di-tert-butyl 2,2'-(anthracene-1,8-diyl)bis(1H-pyrrole-1-carboxylate) **4** as a off-white solid (0.59 g, 78% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46 (s, 1H), 8.01 (d, J = 8.4 Hz, 2H), 7.77 (s, 1H), 7.50-7.45 (m, 4H), 7.42 (d, J = 6.5 Hz, 2H), 6.39-6.37 (m, 2H), 6.27-6.25 (m, 2H), 0.78 (s, 18H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.9, 133.6, 132.0, 131.2, 127.9, 126.1, 124.9, 122.8, 122.0, 115.4, 110.7, 82.6, 27.0. HRMS (ESITOF) m/z $[M + H]^+$ calcd. for $C_{32}H_{33}N_2O_4$ 509.2436, found 509.2436.

1,8-Di(1H-pyrrol-2-yl)anthracene (5): Compound **4** (0.5 g, 0.98 mmol) was dissolved in acetic acid (10 mL) and refluxed at 118 °C under stirring for 2 hours. The solution was cooled to room temperature and quenched with the addition of ice water (10 ml). The resulted precipitate was filtered and washed with water to afford compound **5** as green solid (0.3 g, 98% yield): ^{1}H NMR (400 MHz, Acetone-d6) δ 10.56 (s, 2H), 9.59 (s, 1H), 8.60 (s, 1H), 8.02 (dd, J = 8.5, 4.1 Hz, 2H), 7.54 (s, 2H), 7.53 (d, J = 1.6 Hz, 2H), 7.03 (td, J = 2.6, 1.6 Hz, 2H), 6.60 – 6.56 (m, 2H), 6.32 (dd, J = 5.8, 2.6 Hz, 2H).; ^{13}C NMR (101 MHz, Acetone-d6) δ 126.7, 125.6, 125.3, 124.8, 123.8, 118.7, 109.5, 108.8. MALDI-TOF mass ($C_{22}H_{16}N_2$): 308.81 $[M]^+$.

Macrocycle 3: Samples of compound **5** (100 mg, 0.324 mmol) and pentafluorobenzaldehyde (43.8 µL, 0.324 mmol) in 100 mL of CH_2Cl_2 were stirred under N_2 atmosphere for 15 min. A catalytic amount of TFA (12.4 µL, 0.162 mmol) was added and reaction mixture was stirred for another 5 min. under N_2 atmosphere at room temperature. The oxidant, DDQ (74.02 mg, 0.324 mmol) was added to the reaction mixture and continued stirring for additional 10 min in open air. The crude compound was subjected to basic alumina column chromatography using petroleum ether/CH_2Cl_2 (85:15) and afforded the desired compound **3** as a pink coloured solid in 3% yield (5.0 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.74 (s, 3H), 8.86 (s, 3H), 8.38 (s, 3H), 7.93 (d, J = 8.6 Hz, 6H), 7.64 (d, J = 6.1 Hz, 6H), 7.40 (dd, J = 8.5, 6.9 Hz, 6H), 6.66 (d, J = 4.2 Hz, 6H), 6.57 (d, J = 4.2 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.4, 140.8, 132.5,

131.7, 129.7, 129.1, 127.0, 126.9, 126.0, 125.2, 123.8, 120.9. UV/Vis (Toluene): λ_{max}/nm (log ε): 522 (4.46). HRMS (ESI-TOF) m/z $[M + H]^+$ calcd for $C_{87}H_{40}F_{15}N_6$ 1453.3040, found 1453.3039.





Compound Details

Cpd. 1: C32 H32 N2 O4

Formula	m/z	Observed M/Z	Difference_Da	Difference_PPM	Score
C32 H32 N2 O4	509.2436	509.243603604661	0.158922662251371	0.312694491062241	99.78

Compound Spectra (Zoomed)

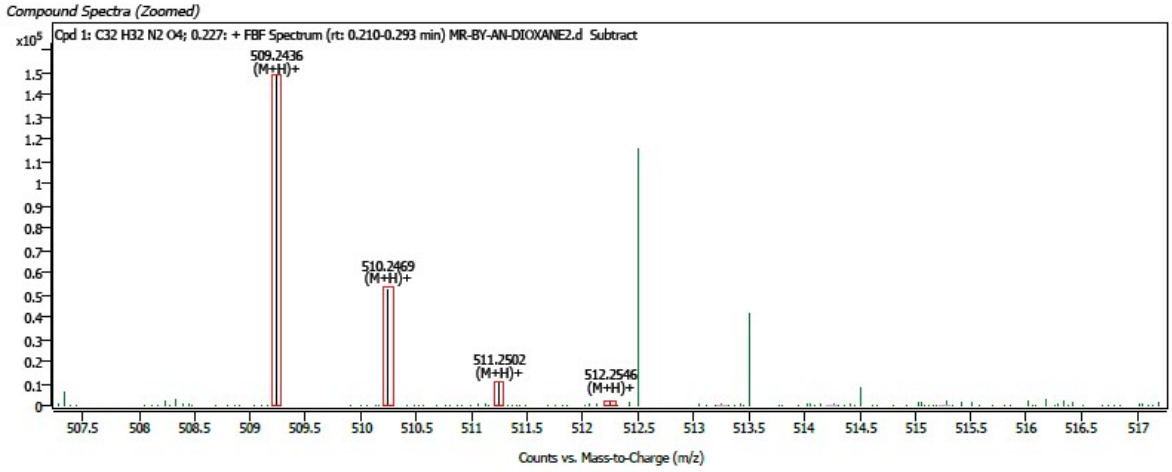


Fig. S1 HR-MS spectrum of the compound **4**.

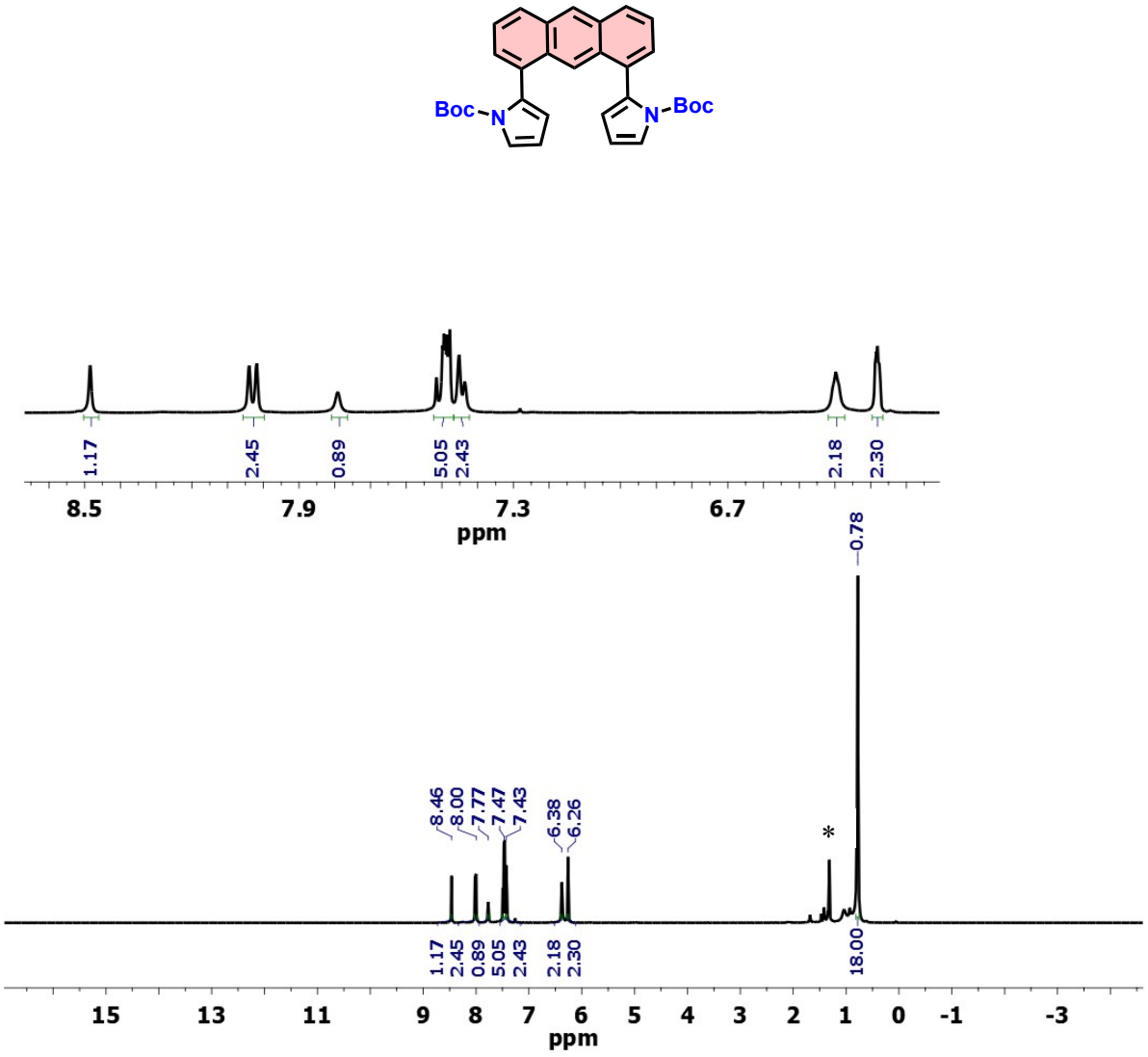


Fig. S2 ^{1}H NMR spectrum of the compound **4** recorded in $CDCl_3$ on 400 MHz FT-NMR spectrometer. Note: Peaks marked with asterisk (*) are due to residual solvents.

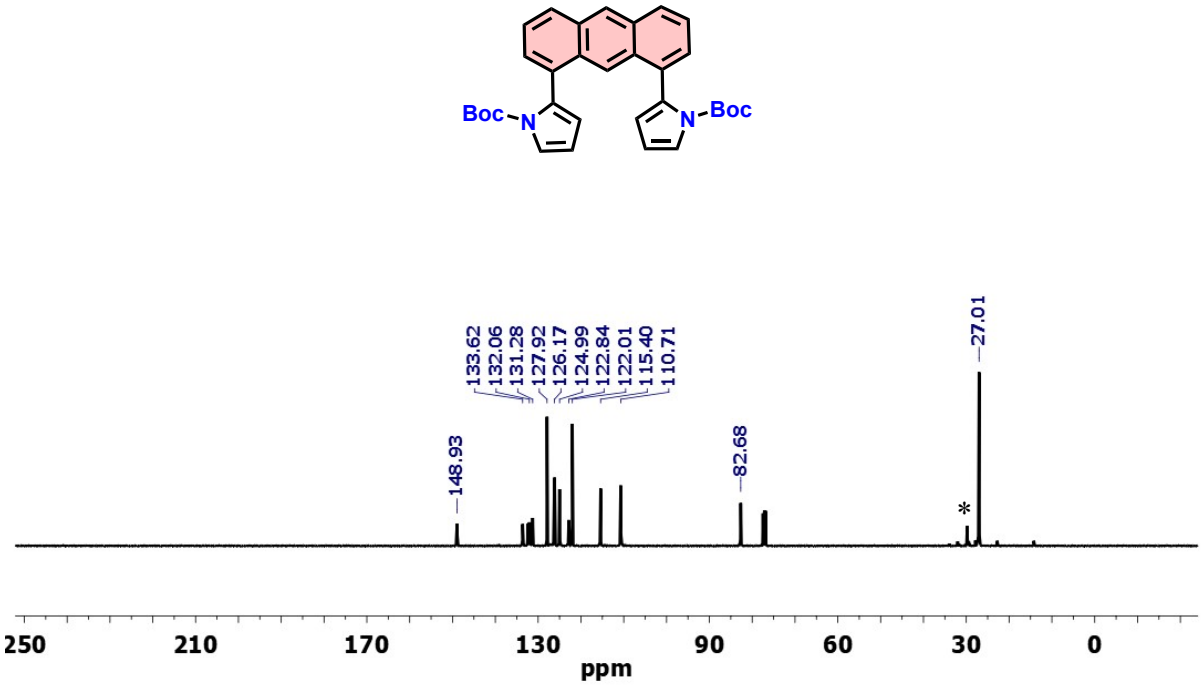
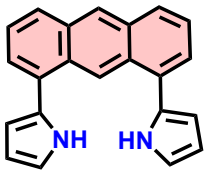
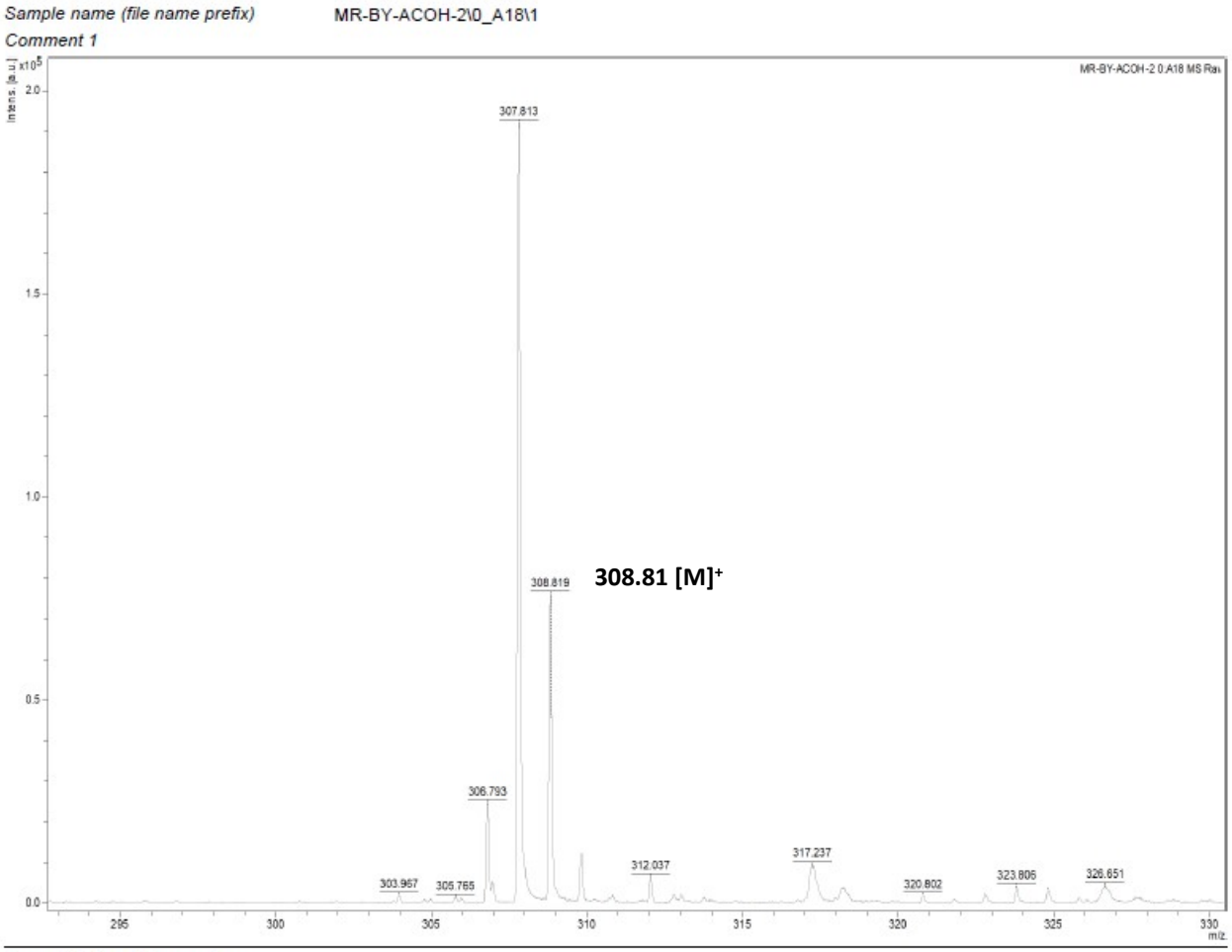


Fig. S3 ^{13}C NMR spectrum of the compound **4** recorded in $CDCl_3$ on 400 MHz FT-NMR spectrometer. Note: Peaks marked with asterisk (*) are due to residual solvents.





Acquisition Parameter

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Aquisition operation mode	Reflector
Voltage polarity	POS
Number of shots	1000
Calibration reference list used	PeptideCalibStandard mono

Fig. S4 MALDI-TOF mass spectrum of the compound **5**.

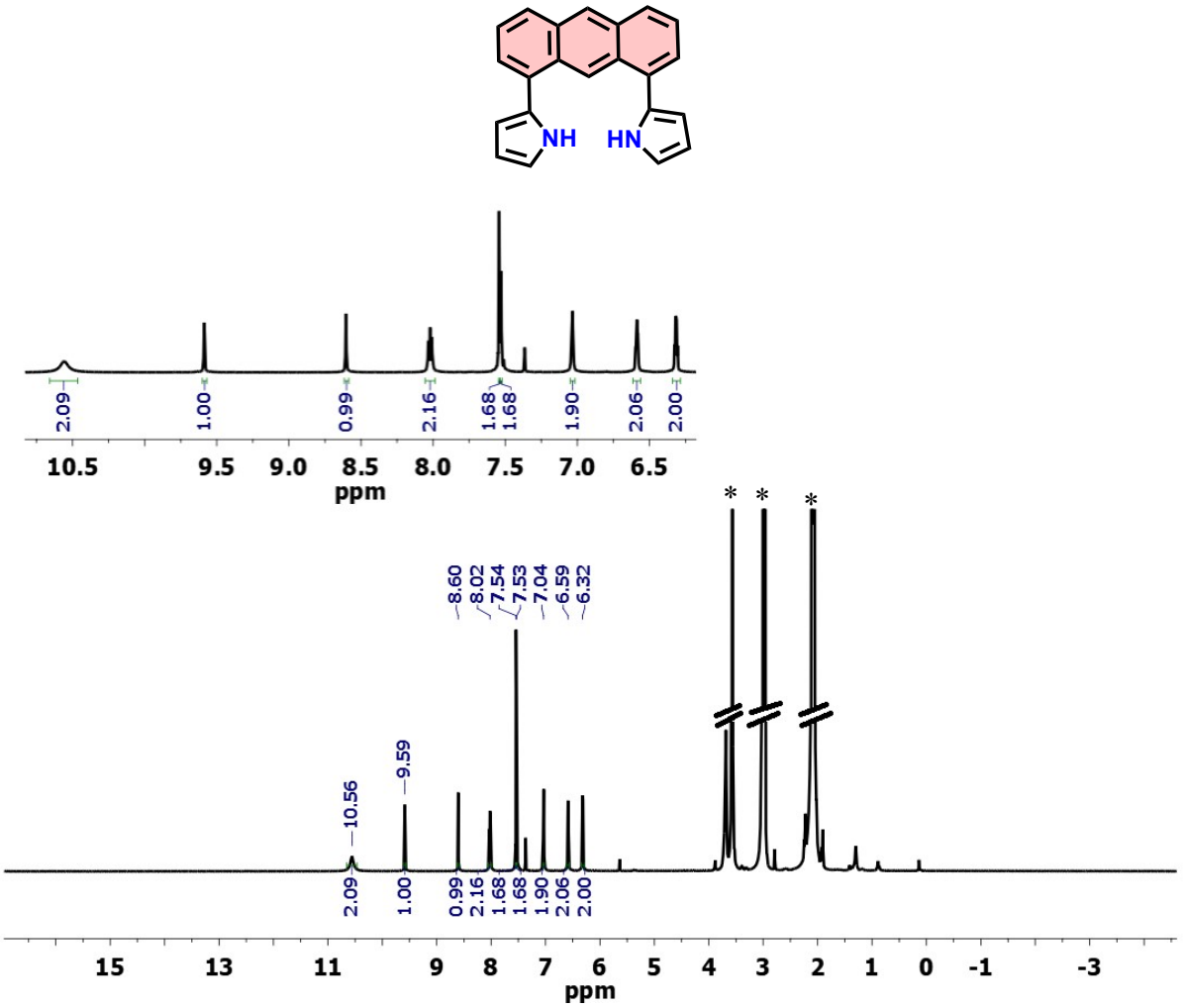

Fig. S5 ^{1}H NMR spectrum of the compound **5** recorded in Acetone-d6 on 400 MHz FT-NMR spectrometer. Peaks marked with asterisk (*) are due to residual solvents

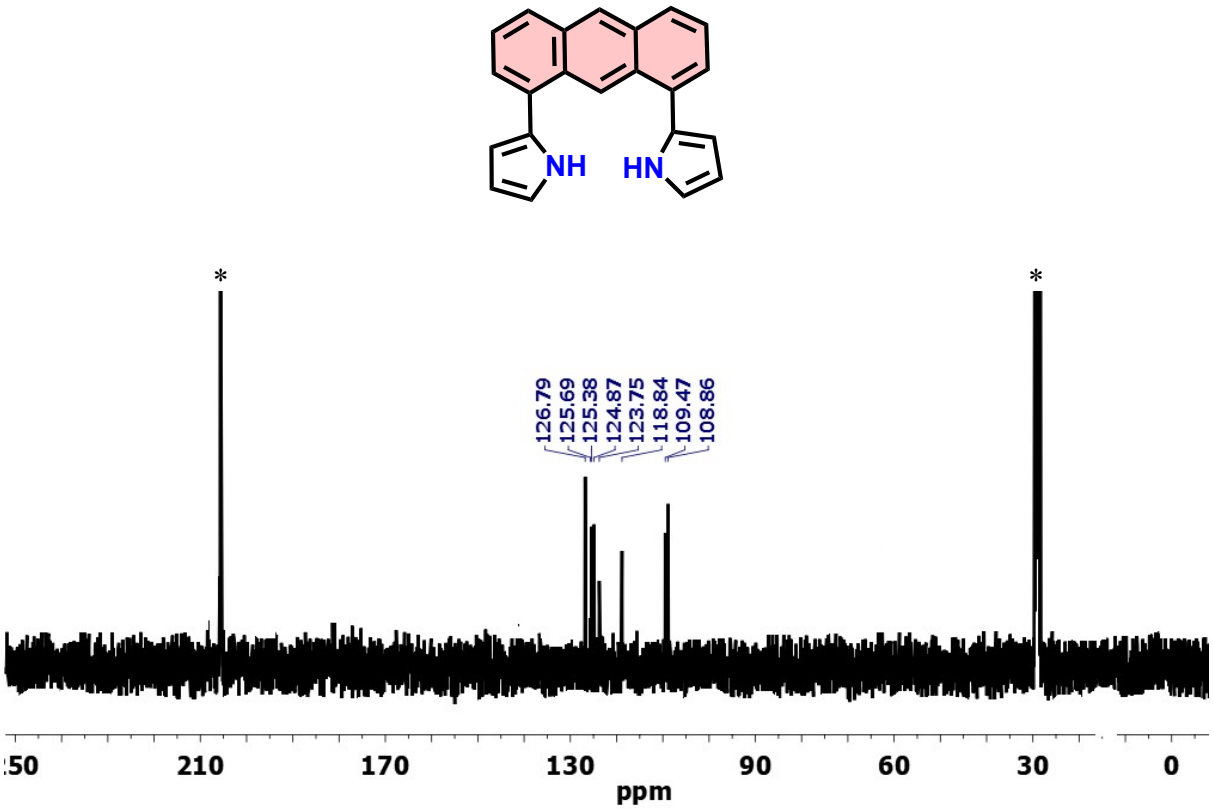

Fig. S6 ^{13}C NMR spectrum of the compound **5** recorded in Acetone-d6 on 400 MHz FT-NMR spectrometer. Peaks marked with asterisk (*) are due to residual solvents

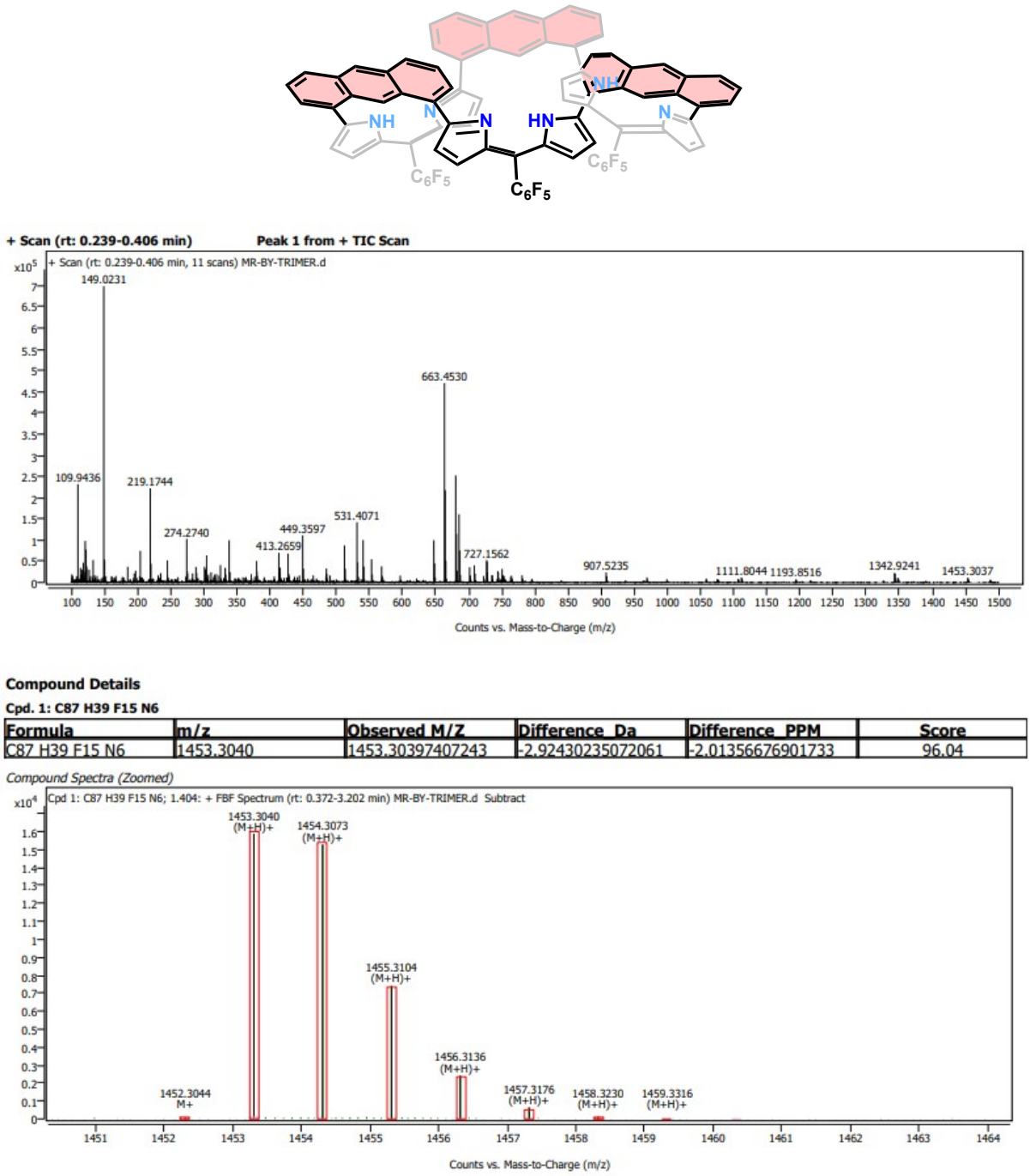

Fig. S7 HR-MS spectrum of the compound **3**.

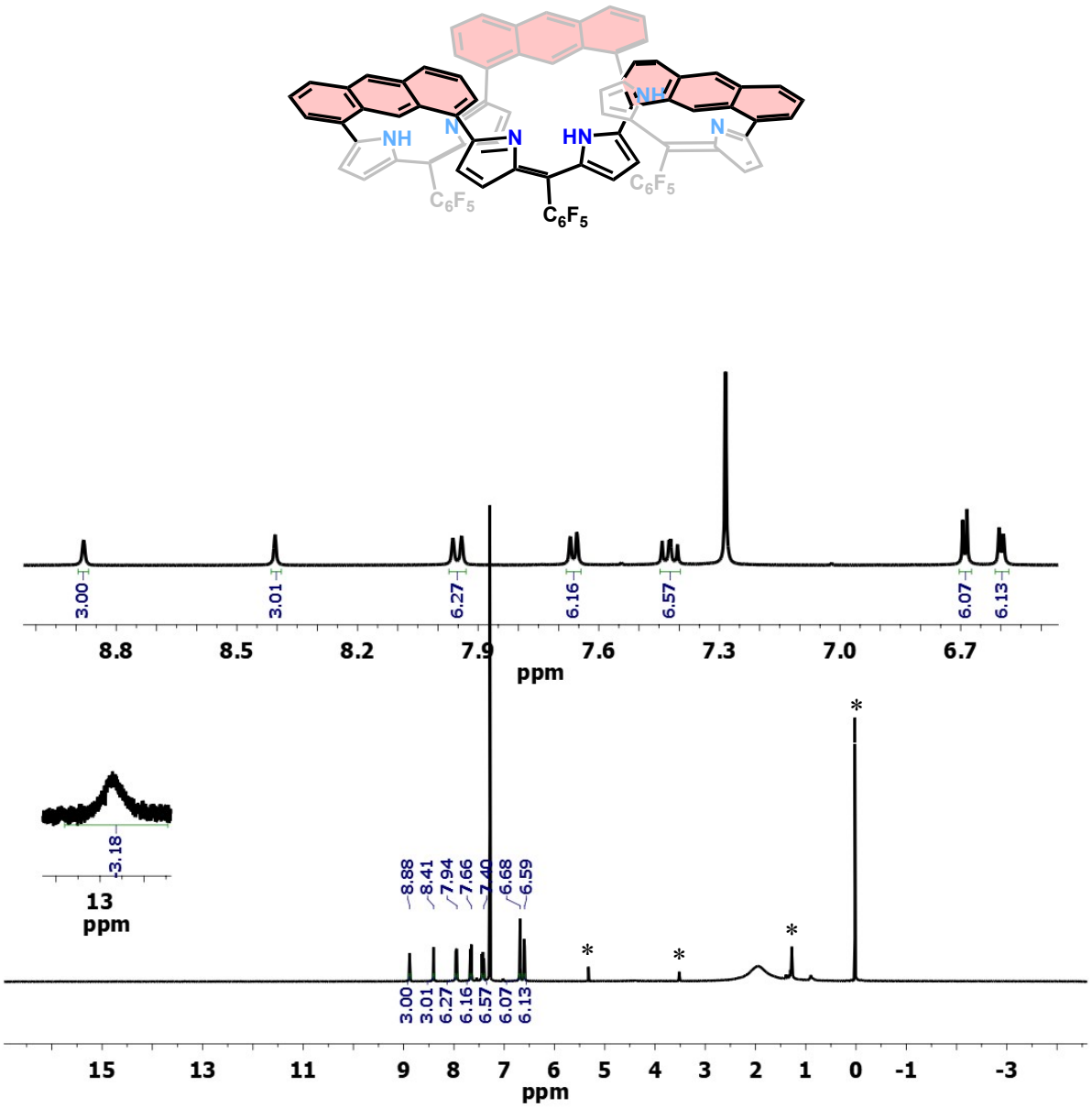

Fig. S8 ^{1}H NMR spectrum of the compound **3** recorded in $CDCl_3$ on 400 MHz FT-NMR spectrometer. Peaks marked with asterisk (*) are due to residual solvents such as Methanol and Dichloromethane.

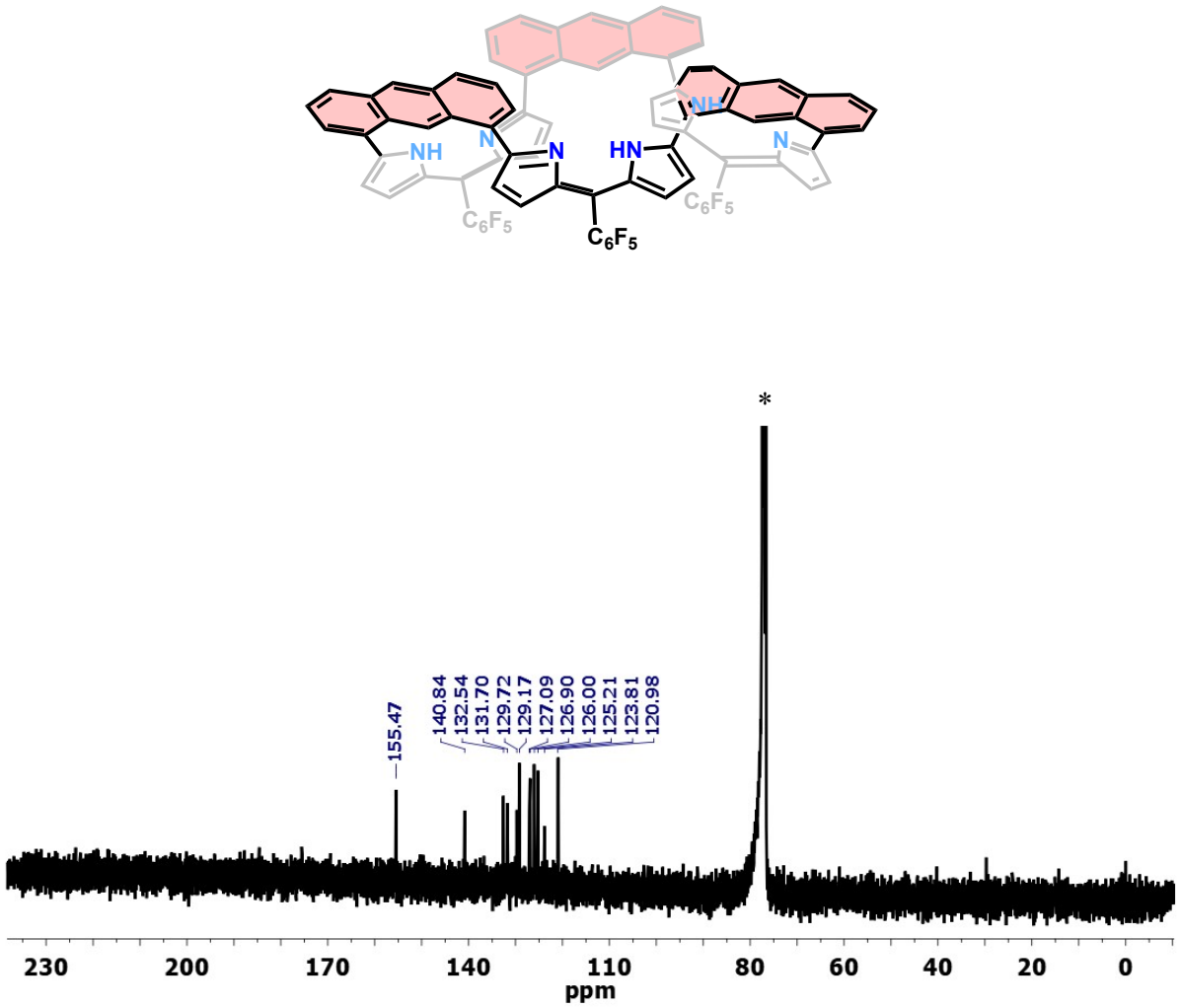

Fig. S9 $^{13}C\{^{1}H\}$ NMR spectrum of the compound **3** recorded in $CDCl_3$ on 400 MHz FT-NMR spectrometer. Peaks marked with asterisk (*) are due to residual solvents

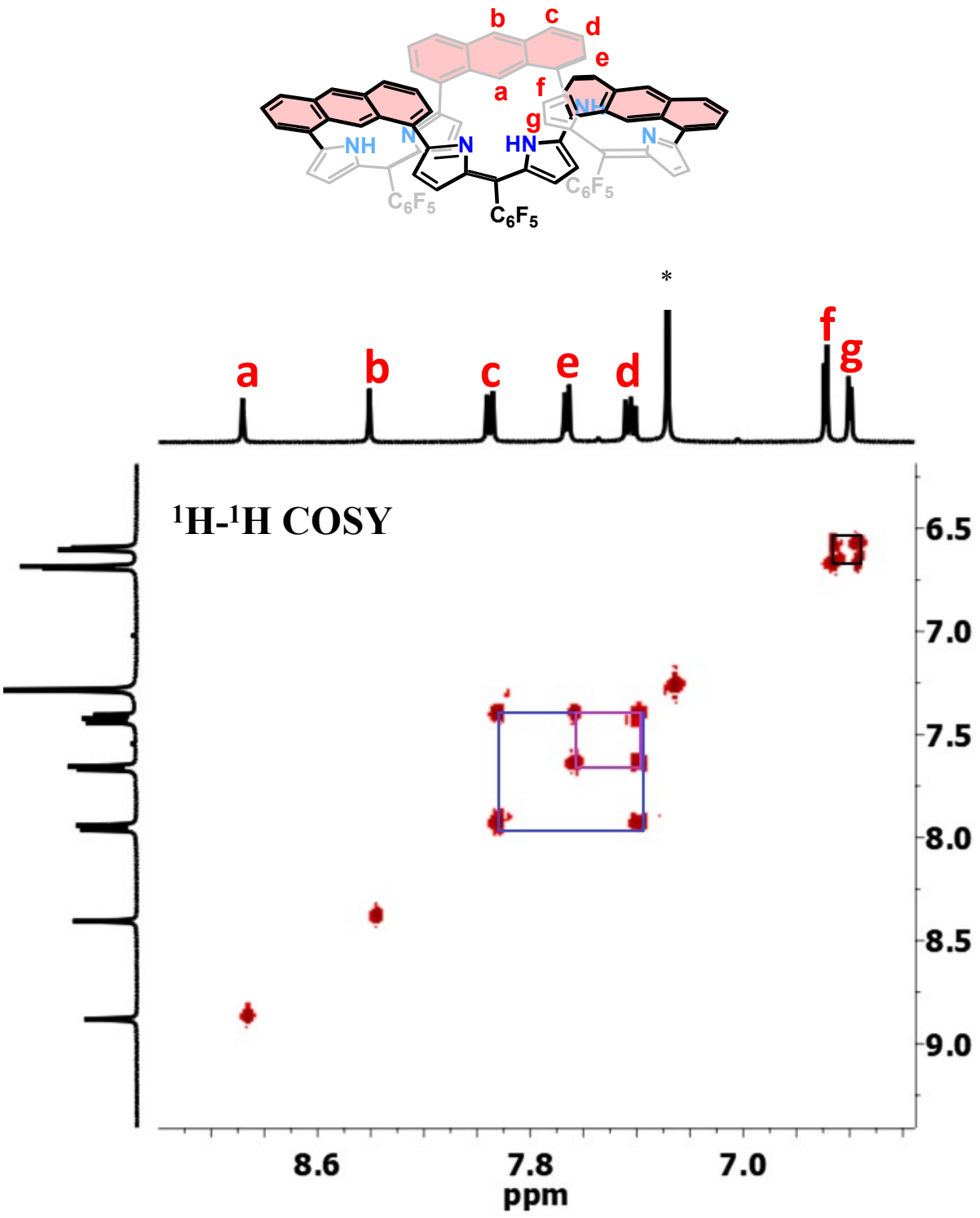

Fig. S10 ^{1}H-^{1}H COSY spectrum of the compound **3** recorded in $CDCl_3$ on 400 MHz NMR instrument. Note: Peaks marked with asterisk (*) are due to residual solvents.

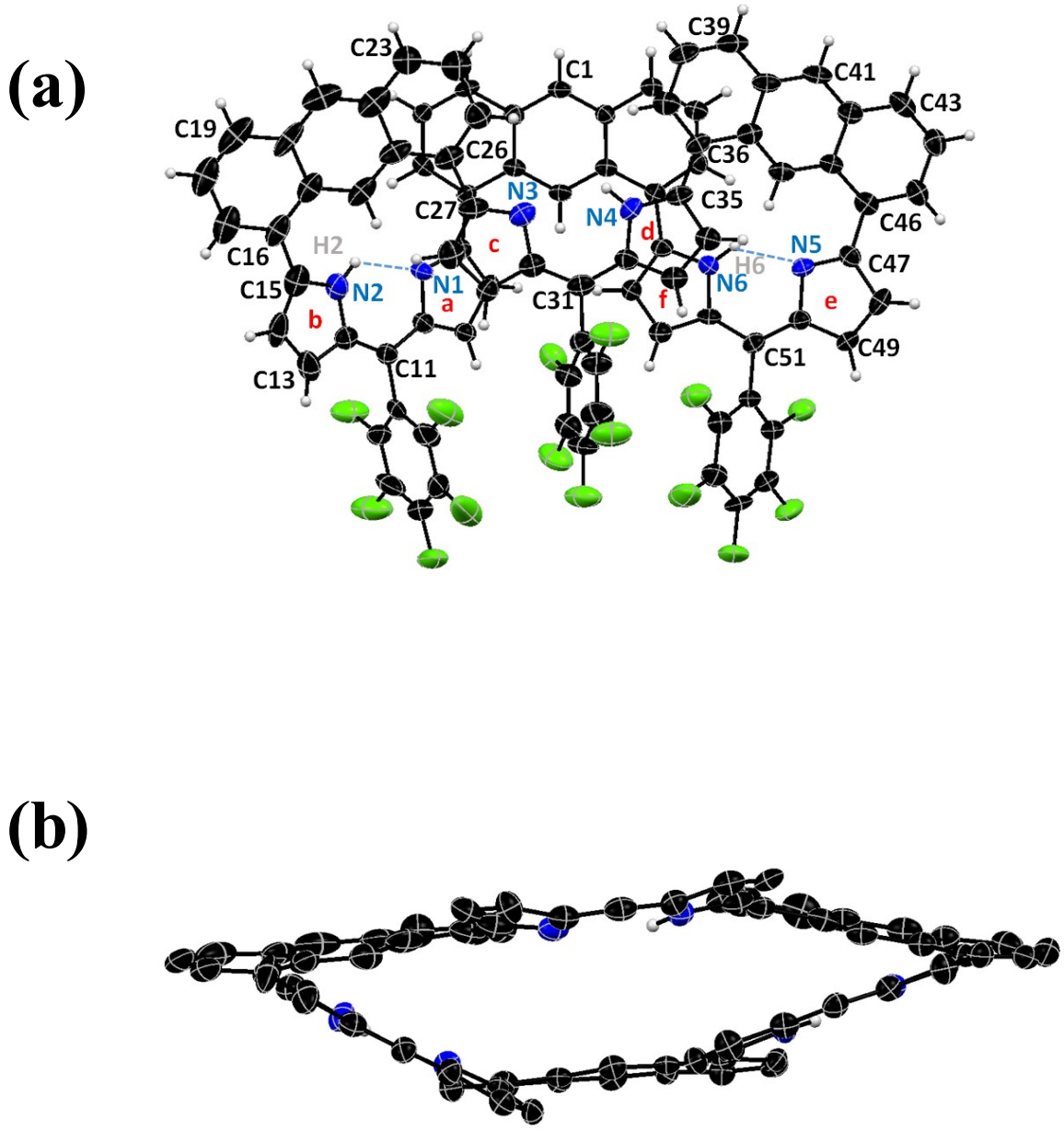

Fig. S11 X-ray crystal structure of macrocycle **3** depicting (a) top and (b) side view (thermal ellipsoid (50% probability). Hydrogen atoms and *meso*-aryl groups have been omitted for clarity.

Table S1. Crystal data and structure refinement for Compound **3**.

Compound	**3**
Empirical Formula	$C_{88}H_{40}Cl_3F_{15}N_6$
Crystal System	monoclinic
Space Group	$P2_1/n$
R_1 ($I > 2.00\sigma(I)$)	0.0960
wR_2 (All reflections)	0.3151
GOF	1.096
a [Å]	19.563 (3)
b [Å]	17.740(3)
c [Å]	21.900(4)
α [°]	90
β [°]	97.679(3)
γ [°]	90
V [$Å^3$]	7533(2)
Z	4
T [K]	105.00
δ_{calc} [g/cm^3]	1.387
F_{000}	3188.2
2θmax [°]	3.76 to 50.14
no. reflns measd. (unique)	122303
no. params.	1012
CCDC no.	2374821

Table S2. Bond lengths for the macrocycle **3**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cl1	C88	1.745(9)	C28	C29	1.402(11)
Cl2	C88	1.749(9)	C29	C30	1.405(10)
Cl3	C88	1.699(9)	C30	C31	1.389(10)
F1	C71	1.353(9)	C31	C32	1.382(10)
F2	C72	1.338(11)	C31	C76	1.494(10)
F3	C73	1.348(10)	C32	C33	1.412(10)
F4	C74	1.349(11)	C33	C34	1.364(10)
F5	C75	1.339(11)	C34	C35	1.431(10)
F6	C77	1.349(9)	C35	C36	1.471(10)
F7	C78	1.341(9)	C36	C37	1.384(10)
F8	C79	1.372(9)	C36	C67	1.446(10)
F9	C80	1.363(9)	C37	C38	1.419(10)
F10	C81	1.353(9)	C38	C39	1.347(11)
F11	C83	1.334(9)	C39	C40	1.407(11)
F12	C84	1.375(10)	C40	C41	1.413(11)
F13	C85	1.349(9)	C40	C67	1.440(9)
F14	C86	1.334(9)	C41	C42	1.382(10)
F15	C87	1.345(8)	C42	C43	1.414(11)
N1	C7	1.378(8)	C42	C69	1.454(10)
N1	C10	1.400(8)	C43	C44	1.348(11)
N2	C12	1.371(9)	C44	C45	1.426(10)
N2	C15	1.322(9)	C45	C46	1.388(10)
N3	C27	1.343(10)	C46	C47	1.461(10)
N3	C30	1.392(9)	C46	C69	1.445(10)
N4	C32	1.391(8)	C47	C48	1.466(10)
N4	C35	1.347(9)	C48	C49	1.359(10)
N5	C47	1.324(9)	C49	C50	1.431(10)
N5	C50	1.401(8)	C50	C51	1.395(10)
N6	C52	1.366(8)	C51	C52	1.426(9)
N6	C55	1.360(8)	C51	C82	1.481(9)
C1	C2	1.393(10)	C52	C53	1.402(10)
C1	C60	1.396(10)	C53	C54	1.383(9)
C2	C3	1.416(9)	C54	C55	1.411(9)
C2	C61	1.437(9)	C55	C56	1.479(9)
C3	C4	1.360(10)	C56	C57	1.377(9)
C4	C5	1.400(9)	C56	C63	1.460(9)
C5	C6	1.359(9)	C57	C58	1.415(9)
C6	C7	1.465(9)	C58	C59	1.336(9)
C6	C61	1.454(9)	C59	C60	1.412(10)
C7	C8	1.382(9)	C60	C63	1.445(9)
C8	C9	1.409(9)	C61	C62	1.387(9)
C9	C10	1.389(10)	C62	C63	1.402(9)
C10	C11	1.413(10)	C64	C65	1.372(11)
C11	C12	1.379(10)	C65	C66	1.386(11)
C11	C70	1.496(10)	C67	C68	1.383(9)
C12	C13	1.441(10)	C68	C69	1.396(10)

C13	C14	1.373(12)	C70	C71	1.370(11)
C14	C15	1.435(11)	C70	C75	1.380(11)
Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
C15	C16	1.483(12)	C71	C72	1.397(11)
C16	C17	1.389(11)	C72	C73	1.374(14)
C16	C64	1.427(12)	C73	C74	1.370(15)
C17	C18	1.445(13)	C74	C75	1.380(13)
C18	C19	1.367(13)	C76	C77	1.391(10)
C19	C20	1.411(13)	C76	C81	1.386(10)
C20	C21	1.426(13)	C77	C78	1.374(11)
C20	C64	1.421(11)	C78	C79	1.351(12)
C21	C22	1.388(13)	C79	C80	1.356(12)
C22	C23	1.415(13)	C80	C81	1.365(11)
C22	C66	1.434(11)	C82	C83	1.390(11)
C23	C24	1.333(13)	C82	C87	1.391(10)
C24	C25	1.424(12)	C83	C84	1.387(11)
C25	C26	1.363(11)	C84	C85	1.328(12)
C26	C27	1.480(11)	C85	C86	1.362(12)
C26	C66	1.447(12)	C86	C87	1.391(10)
C27	C28	1.454(11)			

Table S3. Bond angles for the macrocycle **3**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
Cl2	C88	Cl1	110.8(5)	C50	C49	C48	106.7(7)
Cl3	C88	Cl1	112.1(5)	C49	C50	N5	109.9(6)
Cl3	C88	Cl2	110.7(5)	C51	C50	N5	120.1(6)
C10	N1	C7	109.4(6)	C51	C50	C49	130.0(7)
C15	N2	C12	109.6(7)	C52	C51	C50	123.3(6)
C30	N3	C27	107.4(7)	C82	C51	C50	120.4(6)
C35	N4	C32	109.1(6)	C82	C51	C52	116.3(6)
C50	N5	C47	106.2(6)	C51	C52	N6	122.0(6)
C55	N6	C52	112.3(6)	C53	C52	N6	105.9(6)
C60	C1	C2	123.6(7)	C53	C52	C51	132.0(7)
C3	C2	C1	122.1(7)	C54	C53	C52	107.9(7)
C61	C2	C1	117.4(7)	C55	C54	C53	108.6(7)
C61	C2	C3	120.5(7)	C54	C55	N6	105.2(6)
C4	C3	C2	120.8(7)	C56	C55	N6	119.0(6)
C5	C4	C3	118.9(7)	C56	C55	C54	135.7(7)
C6	C5	C4	123.8(7)	C57	C56	C55	117.9(6)
C7	C6	C5	119.2(6)	C63	C56	C55	124.0(6)
C61	C6	C5	118.9(6)	C63	C56	C57	118.1(6)
C61	C6	C7	121.8(6)	C58	C57	C56	123.5(7)
C6	C7	N1	118.0(6)	C59	C58	C57	118.9(7)
C8	C7	N1	107.6(6)	C60	C59	C58	122.2(7)
C8	C7	C6	134.3(7)	C59	C60	C1	121.8(7)
C9	C8	C7	108.3(6)	C63	C60	C1	118.2(6)
C10	C9	C8	107.8(6)	C63	C60	C59	120.0(7)
C9	C10	N1	106.9(6)	C6	C61	C2	116.8(6)
C11	C10	N1	119.8(7)	C62	C61	C2	120.0(6)
C11	C10	C9	133.3(7)	C62	C61	C6	123.2(6)
C12	C11	C10	125.1(7)	C63	C62	C61	122.1(6)
C70	C11	C10	114.4(7)	C60	C63	C56	117.3(6)
C70	C11	C12	120.5(6)	C62	C63	C56	124.3(6)
C11	C12	N2	121.3(7)	C62	C63	C60	118.4(6)
C13	C12	N2	108.9(7)	C20	C64	C16	118.9(9)
C13	C12	C11	129.7(8)	C65	C64	C16	123.0(8)
C14	C13	C12	104.6(8)	C65	C64	C20	118.0(9)
C15	C14	C13	108.9(8)	C66	C65	C64	124.8(8)
C14	C15	N2	108.0(8)	C26	C66	C22	118.3(9)
C16	C15	N2	122.5(8)	C65	C66	C22	117.8(9)
C16	C15	C14	129.5(8)	C65	C66	C26	123.8(7)

C17	C16	C15	117.0(9)
C64	C16	C15	122.2(8)
Atom	**Atom**	**Atom**	**Angle/°**
C64	C16	C17	120.8(9)
C18	C17	C16	119.6(10)
C19	C18	C17	119.0(10)
C20	C19	C18	122.5(10)
C21	C20	C19	123.1(10)
C64	C20	C19	119.0(10)
C64	C20	C21	117.9(9)
C22	C21	C20	122.8(9)
C23	C22	C21	120.7(10)
C66	C22	C21	118.0(10)
C66	C22	C23	121.3(10)
C24	C23	C22	117.9(10)
C25	C24	C23	122.9(11)
C26	C25	C24	121.3(10)
C27	C26	C25	120.1(9)
C66	C26	C25	118.0(8)
C66	C26	C27	121.8(8)
C26	C27	N3	122.8(8)
C28	C27	N3	110.9(7)
C28	C27	C26	126.2(9)
C29	C28	C27	104.1(8)
C30	C29	C28	108.5(8)
C29	C30	N3	109.0(7)
C31	C30	N3	124.0(7)
C31	C30	C29	126.2(7)
C32	C31	C30	127.5(7)
C76	C31	C30	114.5(7)
C76	C31	C32	117.9(7)
C31	C32	N4	124.4(7)
C33	C32	N4	106.5(7)
C33	C32	C31	129.0(7)
C34	C33	C32	109.4(7)
C35	C34	C33	106.0(7)
C34	C35	N4	108.9(6)
C36	C35	N4	123.7(7)
C36	C35	C34	127.4(7)
C37	C36	C35	119.1(7)
C67	C36	C35	122.1(6)
C67	C36	C37	118.7(7)
C38	C37	C36	121.0(8)
C39	C38	C37	120.7(8)
C40	C39	C38	121.7(8)
C41	C40	C39	124.1(7)
C40	C67	C36	118.9(7)
C68	C67	C36	121.6(7)
Atom	**Atom**	**Atom**	**Angle/°**
C68	C67	C40	119.4(7)
C69	C68	C67	123.5(7)
C46	C69	C42	118.8(7)
C68	C69	C42	117.5(7)
C68	C69	C46	123.6(7)
C71	C70	C11	120.3(7)
C75	C70	C11	122.2(8)
C75	C70	C71	117.2(8)
C70	C71	F1	121.3(7)
C72	C71	F1	116.2(9)
C72	C71	C70	122.5(9)
C71	C72	F2	120.6(10)
C73	C72	F2	120.7(10)
C73	C72	C71	118.7(10)
C72	C73	F3	119.2(12)
C74	C73	F3	121.0(11)
C74	C73	C72	119.7(9)
C73	C74	F4	119.6(11)
C75	C74	F4	120.0(12)
C75	C74	C73	120.4(10)
C70	C75	F5	119.2(8)
C74	C75	F5	119.4(9)
C74	C75	C70	121.4(10)
C77	C76	C31	122.7(7)
C81	C76	C31	122.8(7)
C81	C76	C77	114.5(7)
C76	C77	F6	118.8(7)
C78	C77	F6	117.5(7)
C78	C77	C76	123.7(8)
C77	C78	F7	120.7(8)
C79	C78	F7	120.9(8)
C79	C78	C77	118.4(8)
C78	C79	F8	120.2(8)
C80	C79	F8	118.9(9)
C80	C79	C78	120.9(8)
C79	C80	F9	120.6(8)
C81	C80	F9	119.5(8)
C81	C80	C79	119.9(8)
C76	C81	F10	119.2(7)
C80	C81	F10	118.1(7)
C80	C81	C76	122.7(8)
C83	C82	C51	122.1(7)
C87	C82	C51	122.4(7)

C67	C40	C39	118.8(8)
C67	C40	C41	117.0(7)
Atom	**Atom**	**Atom**	**Angle/°**
C42	C41	C40	123.7(7)
C43	C42	C41	123.4(8)
C69	C42	C41	118.5(7)
C69	C42	C43	118.1(7)
C44	C43	C42	123.2(8)
C45	C44	C43	119.0(8)
C46	C45	C44	122.0(8)
C47	C46	C45	118.4(7)
C69	C46	C45	118.7(7)
C69	C46	C47	122.9(7)
C46	C47	N5	121.0(7)
C48	C47	N5	110.9(7)
C48	C47	C46	128.1(7)
C49	C48	C47	106.2(7)

C87	C82	C83	115.3(7)
C82	C83	F11	119.4(7)
Atom	**Atom**	**Atom**	**Angle/°**
C84	C83	F11	119.6(8)
C84	C83	C82	121.0(8)
C83	C84	F12	117.0(9)
C85	C84	F12	121.1(8)
C85	C84	C83	121.8(9)
C84	C85	F13	121.2(9)
C86	C85	F13	118.8(9)
C86	C85	C84	119.9(8)
C85	C86	F14	120.8(8)
C87	C86	F14	120.2(8)
C87	C86	C85	118.9(8)
C82	C87	F15	120.3(7)
C86	C87	F15	116.8(7)
C86	C87	C82	122.8(8)

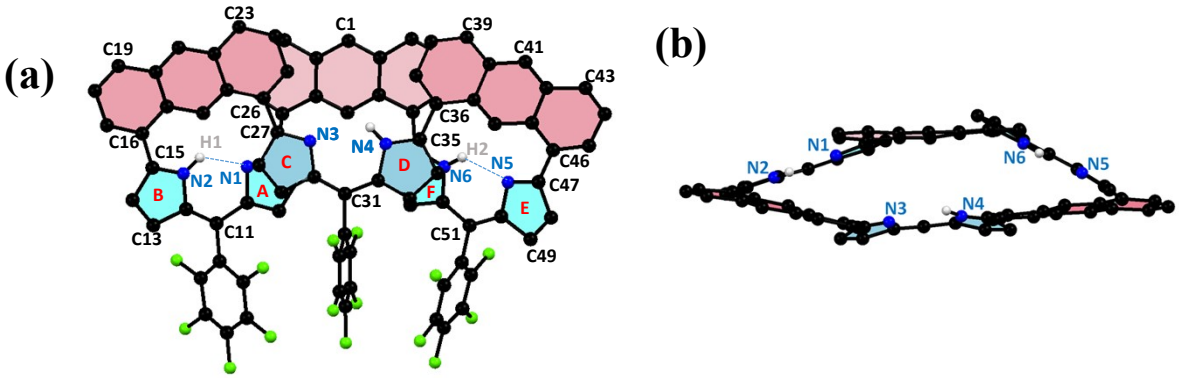

Fig. S12 DFT optimized structures of compound **3** (a) Top view (b) Side view. Hydrogens and *meso*-aryl groups in side view are omitted for clarity.

Figure S13: Cartesian coordinates of the S_0 optimized structures of the compound **3**.
Sum of imaginary frequencies = 0;
Total Free Energy (hartree) with = -5164.7977.

Atom	X	Y	Z
F	-6.318645000	3.669459000	2.393510000
F	0.789452000	1.818495000	-0.447613000
F	-2.579079000	2.875639000	-0.415089000
F	-0.873876000	1.914390000	-4.888890000
F	-6.020474000	6.327177000	2.025111000
F	6.055908000	3.433765000	2.700993000
F	0.837306000	4.505617000	-0.409292000
N	-3.718193000	-0.331463000	2.203840000
F	0.015115000	5.925422000	-2.595231000
N	3.681824000	-0.363117000	2.033157000
H	4.373016000	-0.988120000	1.609141000
F	-3.999159000	7.275641000	0.456412000
N	-5.906843000	-0.296498000	0.634625000
H	-5.237663000	-0.875494000	1.152438000
F	-0.829588000	4.610696000	-4.835452000
N	-1.471485000	-1.740552000	-2.568519000
F	-2.277641000	5.536261000	-0.752847000
N	1.293110000	-1.756892000	-2.463508000
H	0.461119000	-2.330655000	-2.320864000
F	5.932448000	6.114141000	2.362510000
F	3.371804000	2.835803000	-1.156628000
N	5.874431000	-0.544991000	0.475895000
C	2.631033000	-0.653682000	2.847256000
C	-1.235216000	-3.883548000	4.461397000
C	-2.712691000	-0.623201000	3.017281000
C	-1.256114000	-2.583219000	3.829267000
C	2.487611000	-1.993420000	3.426837000
C	3.714354000	0.982119000	1.728773000
C	1.212298000	-3.887086000	4.400998000
C	-5.379753000	-2.737129000	-1.278032000
H	-4.988706000	-1.742597000	-1.130601000
C	-3.314277000	-3.349900000	-2.561142000
C	-1.954620000	0.571608000	3.365524000
H	-1.133471000	0.617509000	4.065649000
F	4.521835000	7.167567000	0.279075000

Atom	X	Y	Z
C	-2.545586000	-1.981492000	3.557995000
C	-3.662240000	1.043717000	1.979377000
C	2.609788000	1.568799000	2.380009000
H	2.348543000	2.616528000	2.351820000
C	-0.031054000	-1.995037000	3.470106000
H	-0.044225000	-1.069212000	2.911286000
C	-2.460359000	-4.548636000	4.766267000
H	-2.416295000	-5.523723000	5.243689000
C	4.765288000	1.565995000	0.968514000
C	-3.697146000	-2.689817000	3.852605000
H	-4.653046000	-2.221407000	3.646868000
C	1.940604000	0.557168000	3.070490000
H	1.086326000	0.680563000	3.715865000
C	1.207502000	-2.589473000	3.761137000
C	-3.661553000	-3.972160000	4.452242000
H	-4.593775000	-4.481077000	4.677580000
C	-4.606357000	1.709270000	1.211402000
C	-5.725133000	1.072659000	0.595096000
C	-7.655284000	0.539508000	-0.465354000
H	-8.571861000	0.587333000	-1.035329000
C	-5.090706000	-5.028376000	-2.070795000
C	-4.597298000	-3.672930000	-1.967231000
C	-0.005095000	-4.490692000	4.727847000
H	0.005519000	-5.476973000	5.185594000
C	-8.787387000	-2.380707000	0.213967000
H	-9.424449000	-1.624532000	0.662243000
C	-7.058243000	-0.644710000	-0.000381000
C	-2.548053000	1.611410000	2.712892000
H	-2.276881000	2.657159000	2.756258000
C	3.635322000	-3.980019000	4.299986000
H	4.576091000	-4.485515000	4.494019000
F	3.241098000	5.511445000	-1.479692000
C	-7.505950000	-2.038011000	-0.164374000
C	-0.093224000	0.278060000	-2.655083000
C	-7.167764000	-4.374680000	-0.942451000
C	-1.326994000	-0.355147000	-2.650306000
C	-2.778770000	-1.978438000	-2.602833000
C	2.446632000	-4.555109000	4.657326000
H	2.419455000	-5.529186000	5.137743000

Atom	X	Y	Z
C	3.649562000	-2.699934000	3.695412000
H	4.609255000	-2.242567000	3.478282000
C	5.823179000	0.849230000	0.425355000
C	-3.538013000	-0.740265000	-2.742499000
H	-4.607606000	-0.652992000	-2.863080000
C	-6.356852000	-5.336132000	-1.556673000
H	-6.728621000	-6.353642000	-1.652702000
C	0.388383000	2.476757000	-1.541963000
C	-4.457123000	3.181188000	1.008384000
C	-6.654392000	-3.035900000	-0.777917000
C	-8.489697000	-4.677262000	-0.494090000
H	-8.860605000	-5.691495000	-0.614836000
C	-2.627807000	0.272522000	-2.747865000
H	-2.822758000	1.332701000	-2.817818000
C	2.608225000	-2.122127000	-2.510300000
C	3.039336000	-3.518419000	-2.407657000
C	-6.822093000	1.605973000	-0.109202000
H	-6.977656000	2.651257000	-0.332966000
C	6.483173000	-3.288876000	-0.821711000
C	-9.280102000	-3.704200000	0.056835000
H	-10.288719000	-3.936288000	0.384884000
C	1.161483000	-0.393302000	-2.633495000
C	-0.049195000	1.770402000	-2.667434000
C	-3.047608000	-5.699921000	-3.198547000
H	-2.433648000	-6.459867000	-3.672828000
C	5.192586000	-2.953812000	-1.254740000
H	4.853540000	-1.942271000	-1.098947000
C	-2.574758000	-4.365172000	-3.139077000
H	-1.620832000	-4.112027000	-3.588573000
C	3.350878000	-0.946021000	-2.744292000
H	4.417901000	-0.897879000	-2.891345000
C	4.756941000	-5.260653000	-1.931414000
C	-5.322369000	4.100749000	1.609497000
C	4.717082000	3.049429000	0.783901000
C	5.360385000	3.921370000	1.666044000
C	-5.179760000	5.474724000	1.429730000
C	-3.434991000	3.701398000	0.207153000
C	7.408985000	-2.306253000	-0.295310000
C	7.015506000	-0.899106000	-0.099009000

Atom	X	Y	Z
C	2.458756000	0.122843000	-2.810222000
H	2.703981000	1.159498000	-2.983593000
C	0.413744000	3.866176000	-1.509065000
C	-0.434327000	3.918124000	-3.760101000
C	-0.451911000	2.525284000	-3.773293000
C	0.002760000	4.591598000	-2.622144000
C	-4.279495000	-6.023772000	-2.693497000
H	-4.659905000	-7.039398000	-2.760380000
C	6.932462000	-4.651686000	-0.977629000
C	8.704267000	-2.689286000	-0.009135000
H	9.402819000	-1.948546000	0.368744000
C	6.042070000	-5.602324000	-1.492488000
H	6.364645000	-6.638043000	-1.569651000
C	-4.147044000	5.961266000	0.631620000
C	4.335239000	-3.879901000	-1.860776000
C	7.013898000	1.356103000	-0.224309000
H	7.244465000	2.396097000	-0.411030000
C	5.304058000	5.303960000	1.503622000
C	7.774508000	0.263196000	-0.532285000
H	8.730856000	0.240505000	-1.037448000
C	8.270296000	-4.993703000	-0.613461000
H	8.593340000	-6.025382000	-0.723838000
C	9.134523000	-4.034572000	-0.155610000
H	10.155317000	-4.296228000	0.106384000
C	-3.270092000	5.070851000	0.017022000
C	2.214553000	-4.521484000	-2.886290000
H	1.255031000	-4.259929000	-3.322008000
C	4.007078000	3.621929000	-0.273268000
C	4.583466000	5.844034000	0.440393000
C	2.612816000	-5.882242000	-2.888196000
H	1.931032000	-6.631653000	-3.278628000
C	3.857609000	-6.243177000	-2.444945000
H	4.181363000	-7.279766000	-2.479414000
C	3.932697000	4.999744000	-0.455495000

TLC Images, Rf value and eluent used :

The R_f value is 0.80 and the solvent used is petroleum ether/CH_2Cl_2 (85:15).

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