General Experimental Methods

All reagents and solvents were of commercial reagent grade and were used without further purification except where noted. Dry THF was obtained by refluxing and distillation over pressed Sodium metal. Column chromatography was performed on silica gel (230-400) in glass columns. ^{1}H NMR and ^{19}F NMR spectra were recorded either on a JEOL 400 MHz or Bruker 500 MHz spectrometer, and chemical shifts were reported as the delta scale in ppm relative to $(CH_3)_2SO$ (´ = 2.50 ppm) or $(CH_3)_2CO$ (´ = 2.1 ppm) as internal reference for ^{1}H. High Resolution Mass spectra were obtained using WATERS G2 Synapt Mass Spectrometer. Electronic spectra were recorded on a Perkin-Elmer »-900 ultraviolet−visible (UV−vis) spectrophotometer. Single crystals were grown in suitable organic solvent and Single crystal X-ray diffraction were performed at 100K on BRUKER KAPPA APEX II CCD Duo diffractometer (operated at 1500 W power: 50 kV, 30 mA) using graphite-monochromated Mo K± radiation (» = 0.71073 Å). Quantum mechanical calculations were carried out on Gaussian 03[12] program suite using High Performance Computing Cluster facility of IISER PUNE. All calculations were carried out by Density Functional Theory (DFT) with Becke's three-parameter hybrid exchange functional and the Lee-Yang-Parr correlation functional (B3LYP) and 6-31G(d,p) basis set for all the atoms were employed in the calculations. To estimate the NICS(0) values at the centre of the seven membered rings of molecular plane of all the macrocycles, the gauge independent atomic orbital (GIAO) method used based on the optimized geometries. The molecular structures obtained from single crystal analysis were used for geometry optimization. Cyclic voltammetry (CV) and Differential pulse voltammetry (DPV) measurements were carried out on a BAS electrochemical system using a conventional three-electrode cell in dry CH_2Cl_2 containing 0.1 M tetrabutylammonium perchlorate (TBAP) as the supporting electrolyte. Measurements were carried out under an Ar atmosphere. A glassy carbon (working electrode), a platinum wire (counter electrode), and saturated calomel (reference electrode) were used.

Reference:

13. Gaussian 03, Revision C.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.

Procedure for Synthesis 4: *Meso*-pentafluorophenyl doubly N-confused dipyrromethane (DNCDPM) was synthesized as per literature procedure. To a DNCDPM (300 mg, 0.9615 mmol, 1 equiv.), 10ml dry THF was added under N_2 inert atmosphere followed by addition of DDQ (480 mg, 2.1154 mmol, 2.2 equiv.). After stirring reaction mixture for one hour, copper(II) acetate (173 mg, 0.9615 mmol, 1 equiv.) was added and the reaction mixture was stirred for overnight. Reaction was quenched with 100ml distilled water and organic phase was extracted thrice with dichloromethane. The combined dichloromethane extracts was washed with water, dried over Na_2SO_4 and evaporated under vacuo. The crude product was purified by silica gel column chromatography using hexane/ethyl acetate as the eluent and pink color solution obtained as **4** (12mg, 4%).
It has been found that, this compound has poor solubility in common organic solvents hence hampered the ^{13}C-NMR studies.

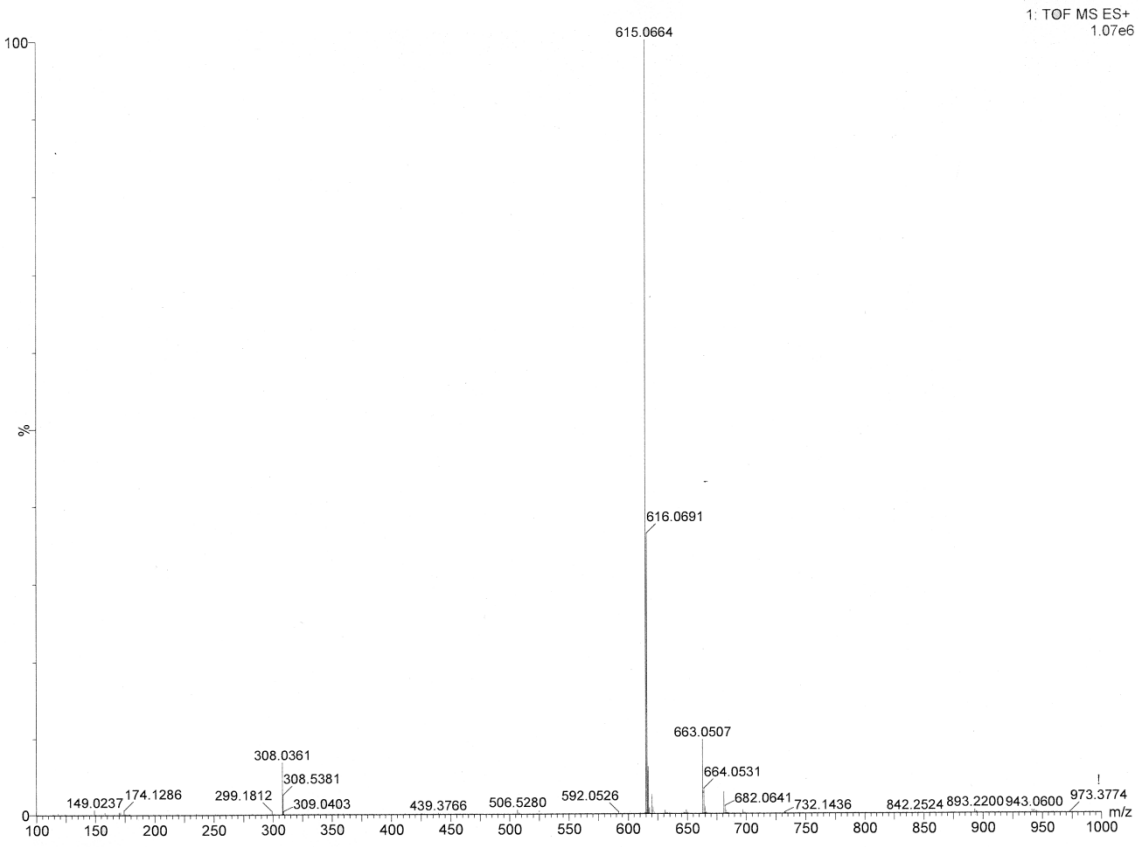
^{1}H-NMR (Acetone-d_6, 400MHz, 295K) ´ = 6.84 (d, J = 4.0 Hz, 2H), 7.79 (d, J = 4.0 Hz, 2H), 7.96 (d, J = 4.0 Hz, 2H), 9.53 (d, J = 4.0 Hz, 2H). **^{19}F-NMR** (Acetone-d_6, 376MHz, 295K) ´ = -141.62 (d, J = 11.28 Hz, 4F), -153.93 (t, J = 15.04 Hz, 2F), -162.07 (t, J = 15.04 Hz, 4F). **UV-Vis** (CH_2Cl_2): »$_{max}$(µ)L mol^{-1}cm^{-1} = 262 nm(17,800), 280 nm(17,800), 361 nm(10,000) and 514 nm(6,700). **HRMS** *m/z* calcd. for $(C_{30}H_8N_4F_{10}+H)^+$ = 615.0668, Observed = 615.0664. **Crystal data:** $C_{30}H_8N_4F_{10}$ (M_r = 614.40), triclinic, space group *P-1 (No.2)*, *a* = 5.996(2), *b* = 7.348(3), *c* = 13.198(5)Å, ± = 87.325(8), ² = 86.010(8), ³ = 71.490(8)°, V = 549.9(4)Å^3, Z = 1, $Á_{calcd}$ = 1.855 mg/m^3, *T* = 100K, R_{int} (all data) = 0.0385, R_1(all data) = 0.0576, R_W (all data) = 0.1124, GOF = 1.043

Procedure for Synthesis 5: DNCDPM (100 mg, 0.3205 mmol, 1 equiv.) were dissolved in 100ml dry THF under inert atmosphere of N_2 and DDQ (160 mg, 0.7051 mmol, 2.2 equiv) was added. After one hour, Iron(III) acetylacetonoate (113 mg, 0.3205 mmol, 1 equiv.) was added and the reaction mixture stirred overnight. Furthermore, reaction mixture was passed through bed of basic alumina. The first fraction afforded pink color solution of **4** (5mg, 5%) in dichlormethane and second fraction provided dark color solution in methanol/dichloromethane combination which was further purified by silica gel column chromatography using hexane/ethyl acetate as a eluent to give greenish yellow color solution as **5** (10 mg, 10%).

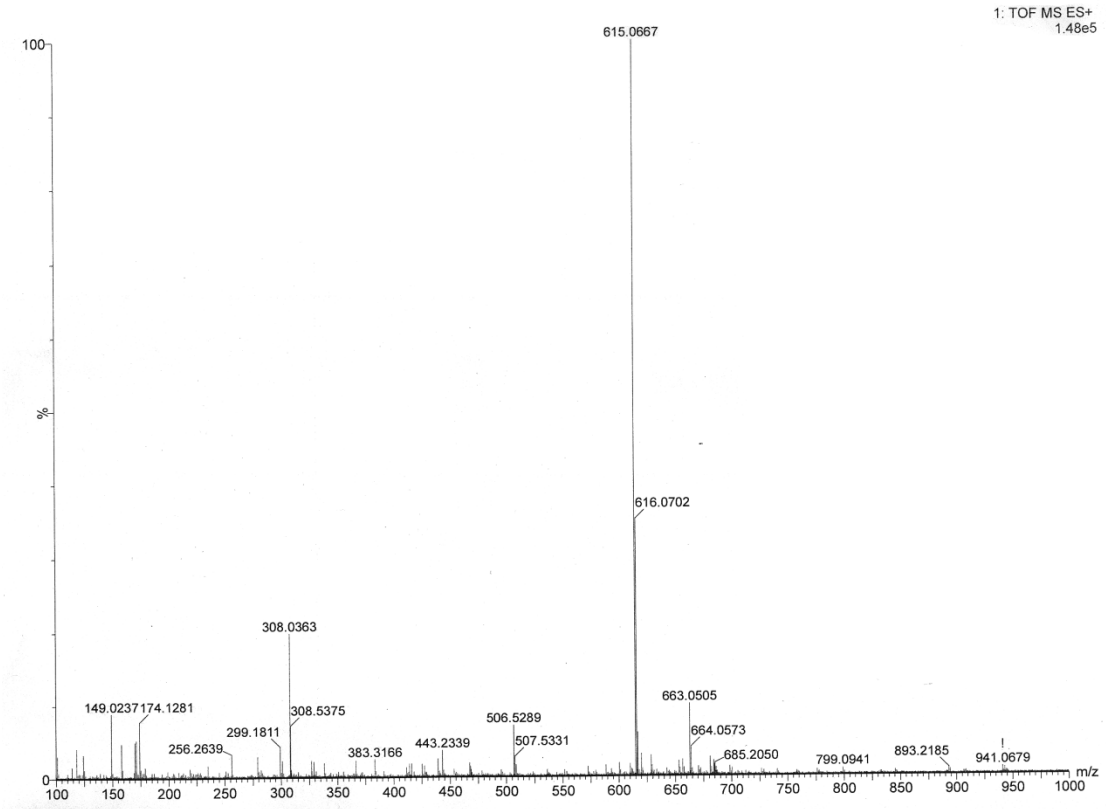
^{1}H-NMR (DMSO-d_6, 400MHz, 295K) ´ = 6.28 (d, J = 4.0 Hz, 1H), 6.73 (d, J = 4.0 Hz, 1H), 7.19 (d, J = 4.0 Hz, 1H), 7.50 (d, J = 4.0 Hz, 1H), 7.82 (d, J = 4.0 Hz, 1H), 8.71 (s, 1H), 9.28 (d, J = 4.0 Hz, 1H), 13.46 (bs, 1H, exchangeable with D_2O). **^{19}F-NMR** (DMSO-d_6, 376MHz, 295K) ´ = -142.41 (d, J = 22.56 Hz, 4F), -155.63 (td, J = 15.04 Hz, 2F), -162.89 (td, J = 15.04 Hz, 4F). **UV-Vis** (CH_2Cl_2): »$_{max}$(µ)L mol^{-1}cm^{-1} = 268 nm (32,600) 282 nm(32,500), 346 nm(33,600) and 451 nm(8,800). **HRMS** *m/z* calcd. for $(C_{30}H_8N_4F_{10}+H)^+$ = 615.0668, Observed = 615.0667. **Crystal data:** $C_{30}H_8N_4F_{10}O_1$ (M_r = 630.40), monoclinic, space group *P21/c (No.14)*, *a* = 28.021(12), *b* = 11.565(3), *c* = 7.319(3)Å, ± = 90.00, ² = 95.576(10), ³ = 90.00°, V = 2360.6(17)Å^3, Z = 4, $Á_{calcd}$ = 1.774 mg/m^3, *T* = 100K, R_{int} (all data) = 0.0793, R_1(all data) = 0.1812, R_W (all data) = 0.2303, GOF = 1.112.

Procedure for Synthesis Me-5: To a **5** (100 mg, 0.1628 mmole, 1 equiv.) in 5 ml dry dimethyl formamide under N_2 inert atmosphere, sodium hydride(1 equiv.) was added at 0^{oc}. After 30 minute, methyl iodide (1.5 equiv.) was added and reaction mixture brought to room temperature. Reaction mixture quenched with ice cold distilled water and organic compound was extracted with ethyl acetate from ice cold reaction mixture. The organic layer was evaporated on rota evaporator to get crude solid which was further purified on silica gel in ethyl acetate/n-hexane combination to get yellowish colored compound **Me-5** (55 mg ,54%).

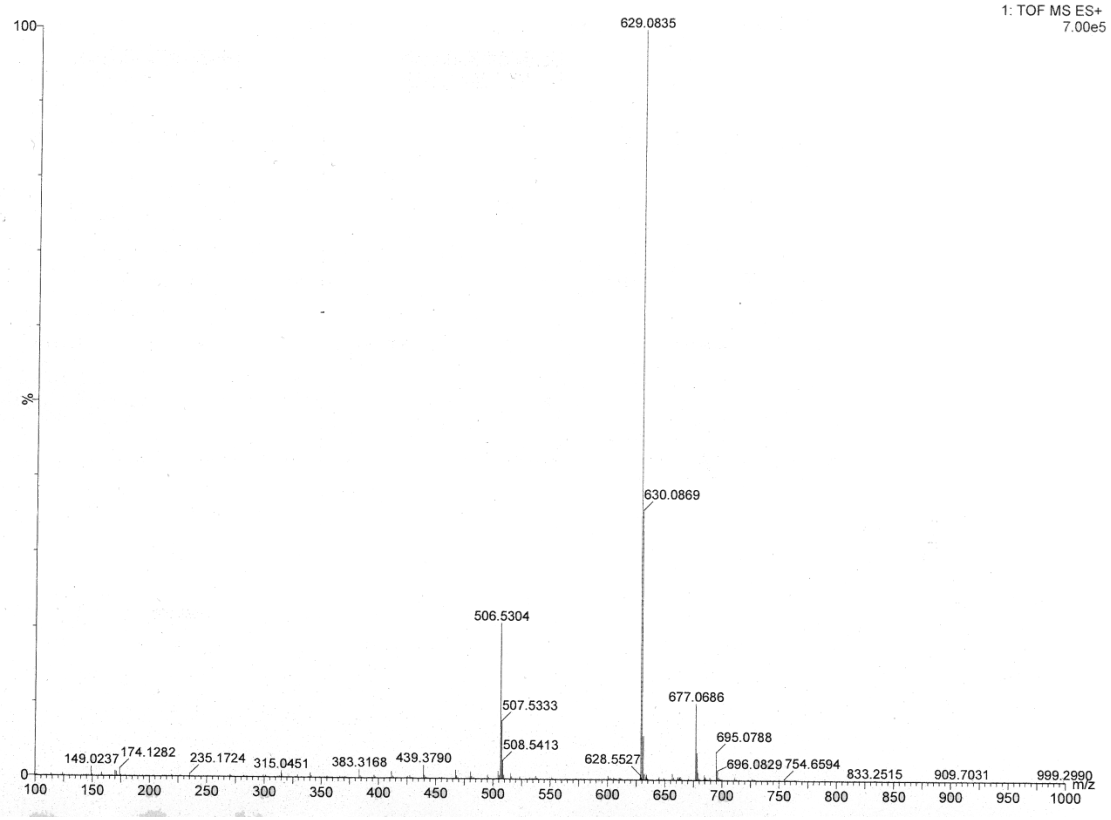
^{1}H-NMR (Acetone-d_6, 400MHz, 295K) ´ = 4.75 (s, 3H), 6.28 (d, J = 4.0 Hz, 1H), 6.72 (d, J = 4.0 Hz, 1H), 7.21 (d, J = 4.0 Hz, 1H), 7.42 (d, J = 4.0 Hz, 1H), 7.77 (d, J = 4.0 Hz, 1H), 8.66 (s, 1H), 9.35 (s, 1H). **^{19}F-NMR** (Acetone-d_6, 376MHz, 295K) ´ = -140.01 (d, J = 76.96 Hz, 4F), -152.84 (d, J = 221.84 Hz, 2F), -160.65 (d, J = 206.80 Hz, 4F). **UV-Vis** (CH_2Cl_2): »$_{max}$(µ)L mol-1cm-1 = 261 nm(43,900), 285 nm(38,700) 351 nm(51,200) and 465 nm(13,000). **HRMS** m/z calcd. for $(C_{31}H_{10}N_4F_{10}+H)^+$= 629.0824, Observed = 629.0835. **Crystal data**: $C_{31}H_{10}N_4F_{10}$ (Mr = 628.43), triclinic, space group P 1 (No.1), a = 6.1461(11), b = 7.3648(13), c = 14.031(3)Å, ± = 76.834(4), ² = 82.082(4), ³ = 72.763(4)°, V = 589.0(2)Å^3, Z = 1, Ácalcd = 1.772 mg/m3, T = 100K, Rint (all data) = 0.0484, R1(all data) = 0.0927, RW (all data) = 0.1616, GOF = 0.963



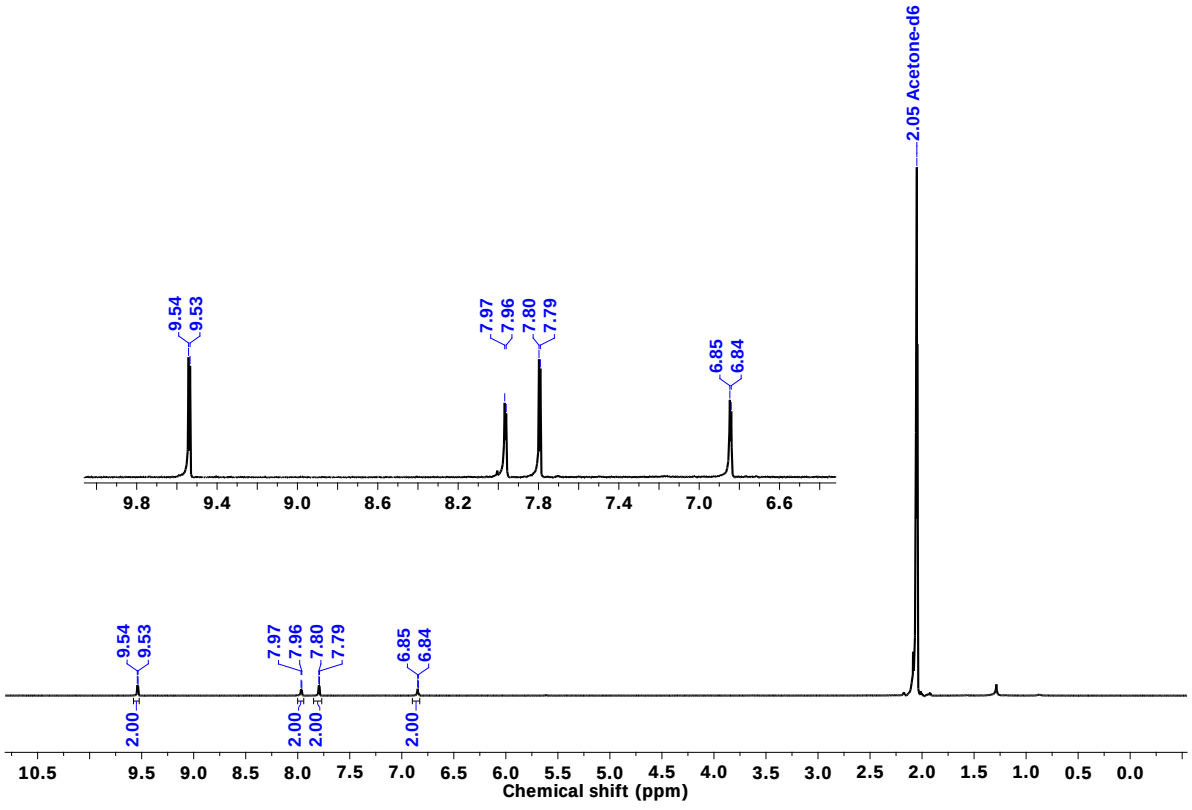
S1: HR-ESI-TOF mass spectrum of **4**.



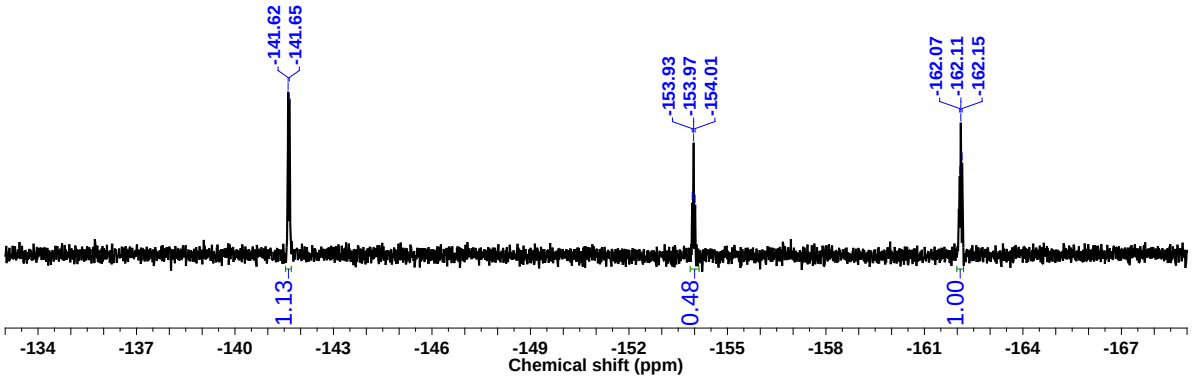
S2: HR-ESI-TOF mass spectrum of **5**.



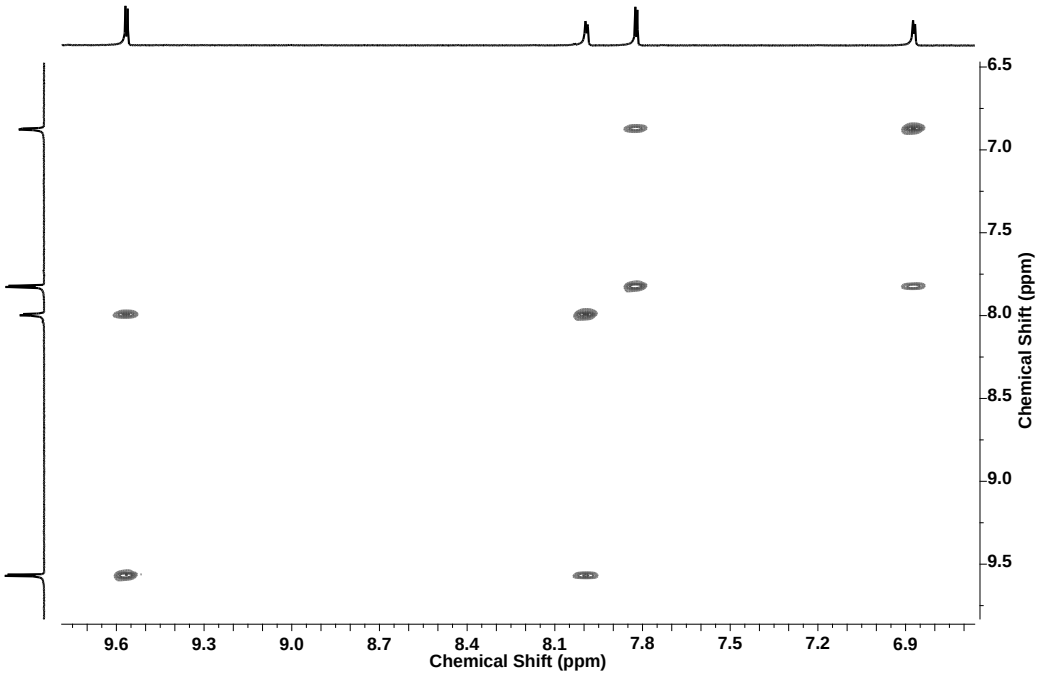
S3: HR-ESI-TOF mass spectrum of **Me-5**.



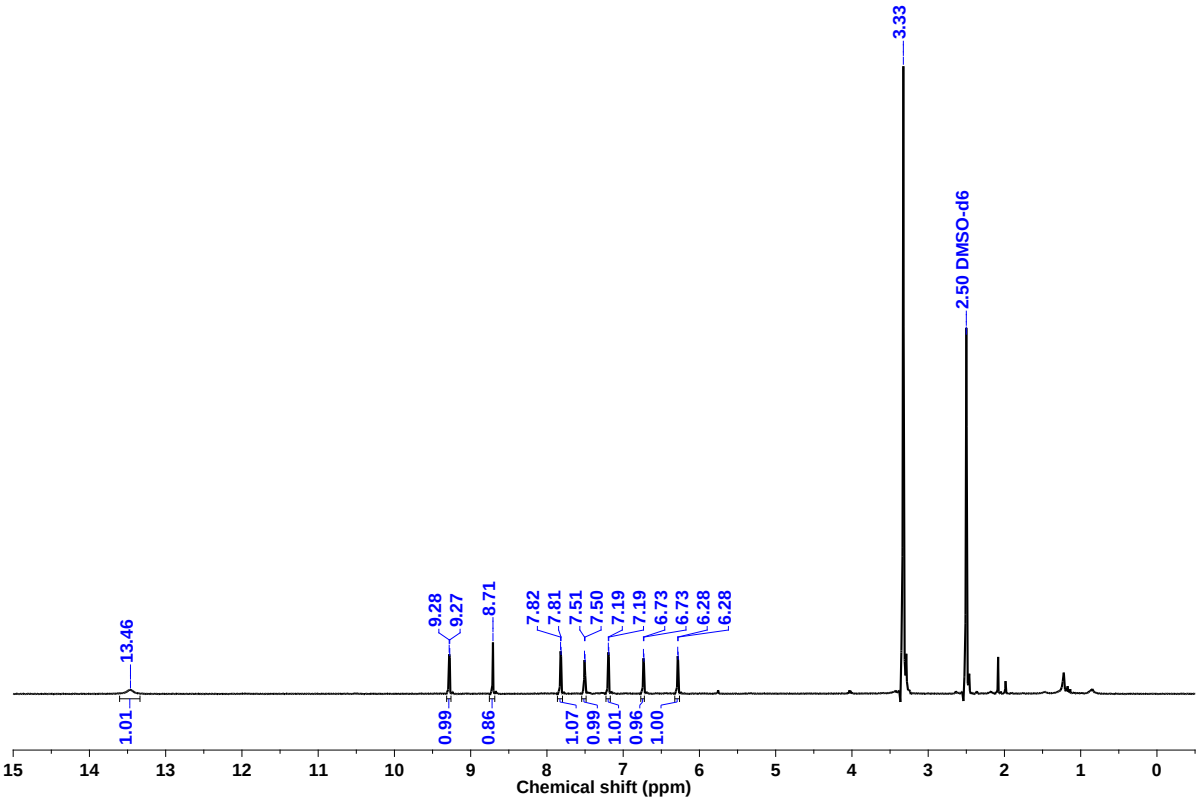
S4: ^{1}H-NMR spectrum of **4** in *Acetone-d_6* at 295K.



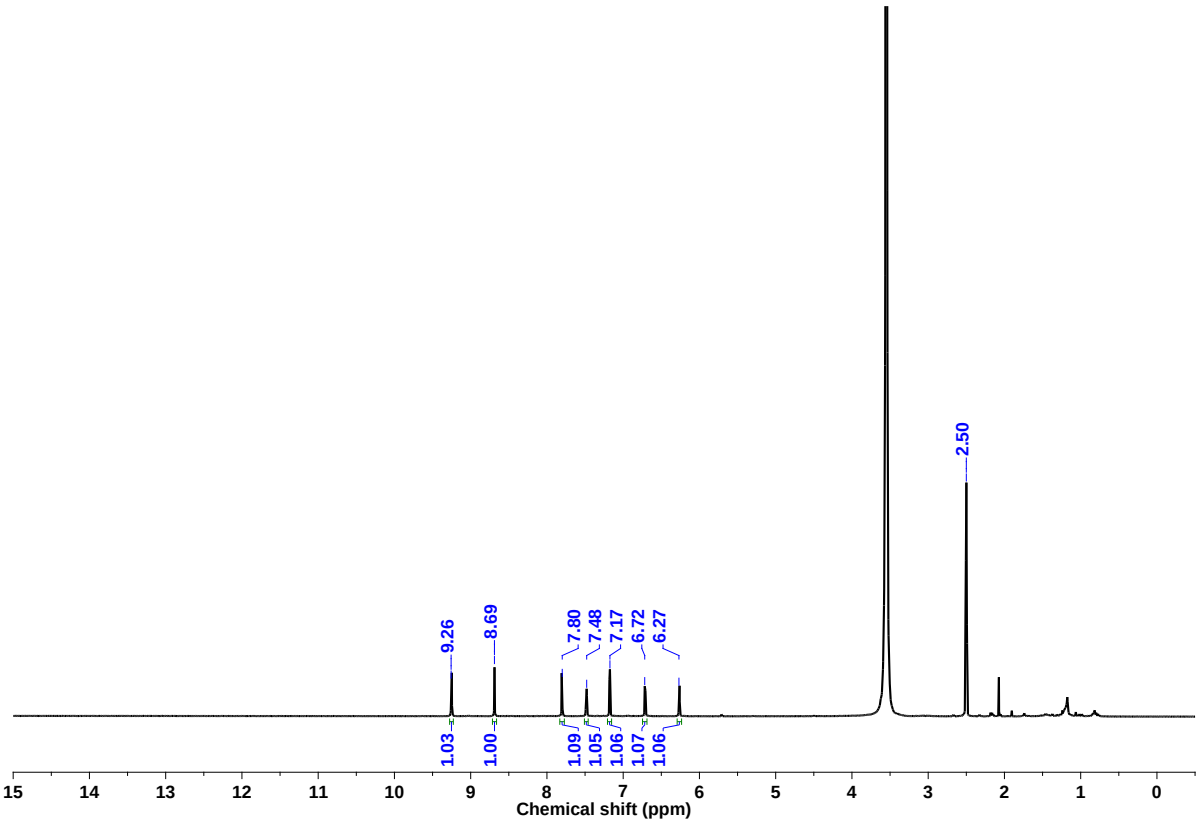
S5: ^{19}F-NMR spectrum of **4** in *Acetone-d*$_6$ at 295K.



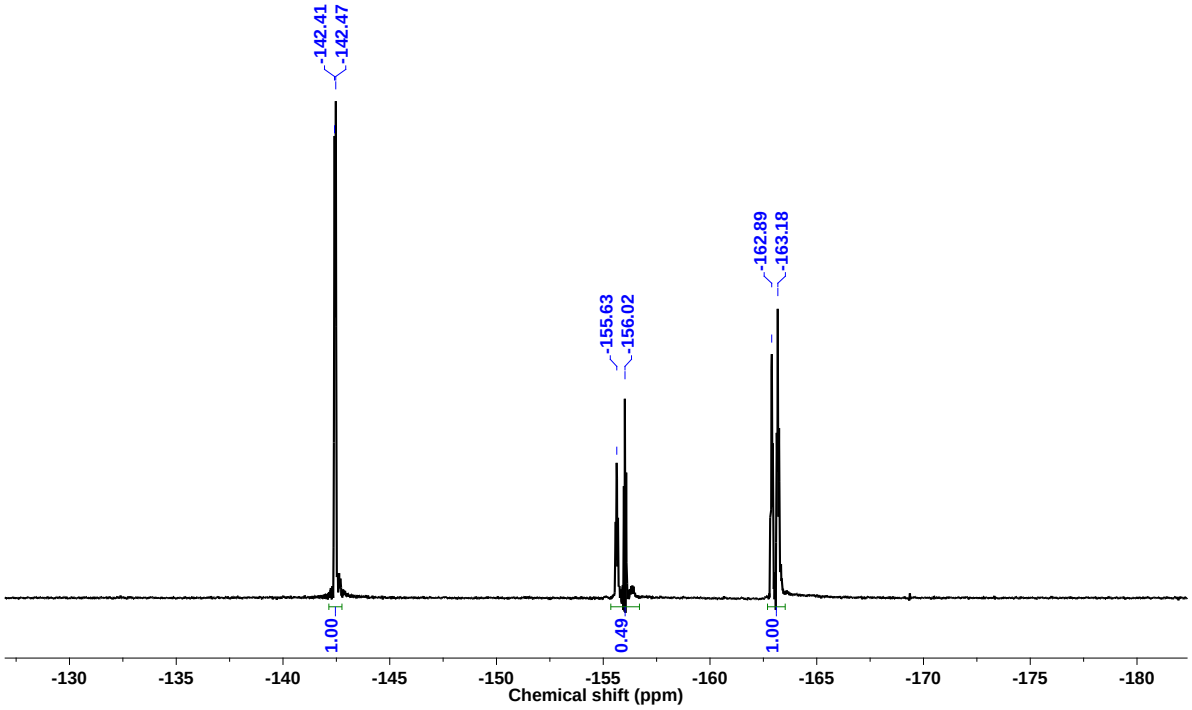
S6: ^{1}H-^{1}H COSY spectrum of **4** in *Acetone-d*$_6$ at 295K.



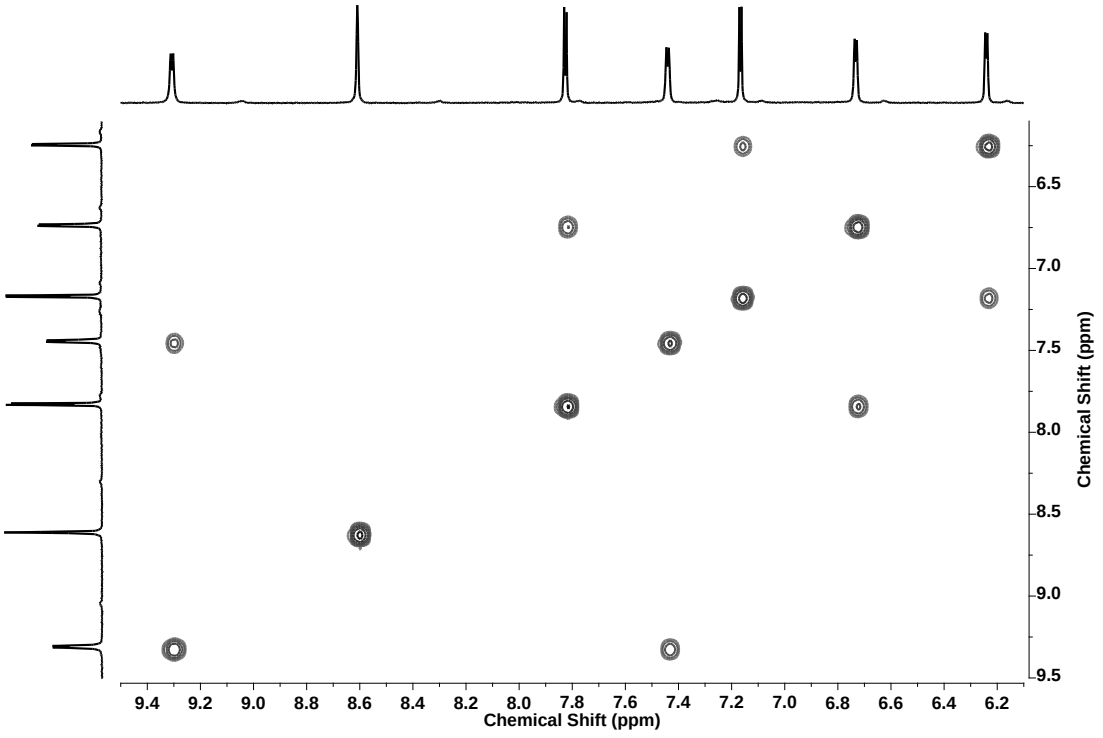
S7: ^{1}H-NMR spectrum of **5** in *Dimethyl Sulphoxide-d_6* at 295K.



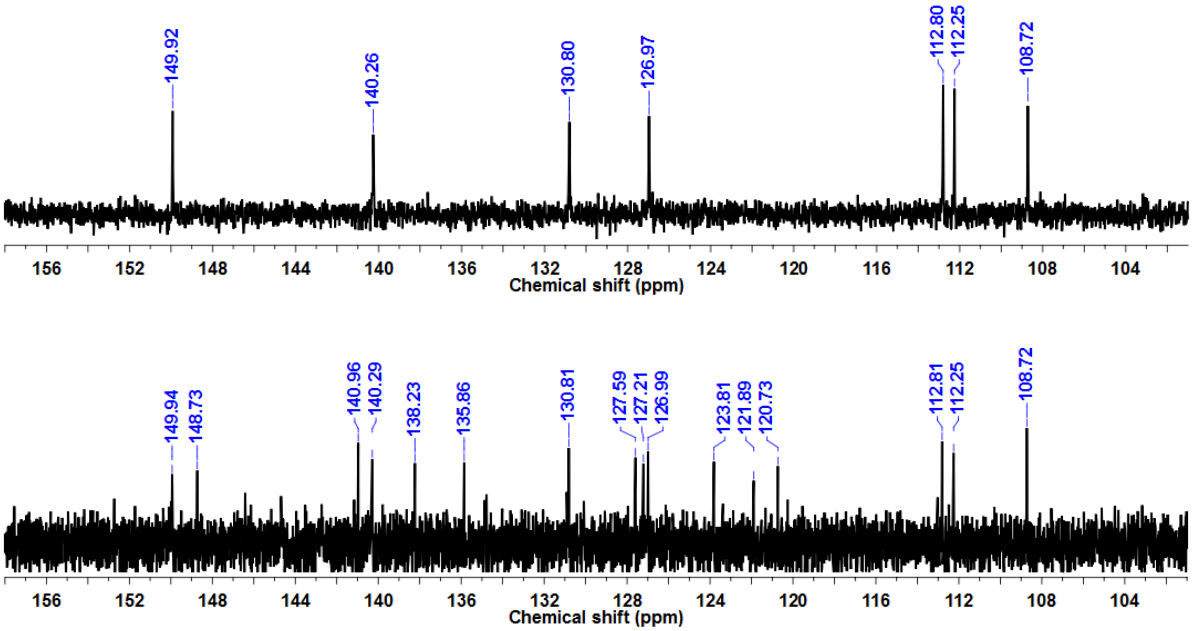
S8: ^{1}H-NMR spectrum of **5** after D_2O exchange in *Dimethyl Sulphoxide-d_6* at 295K.



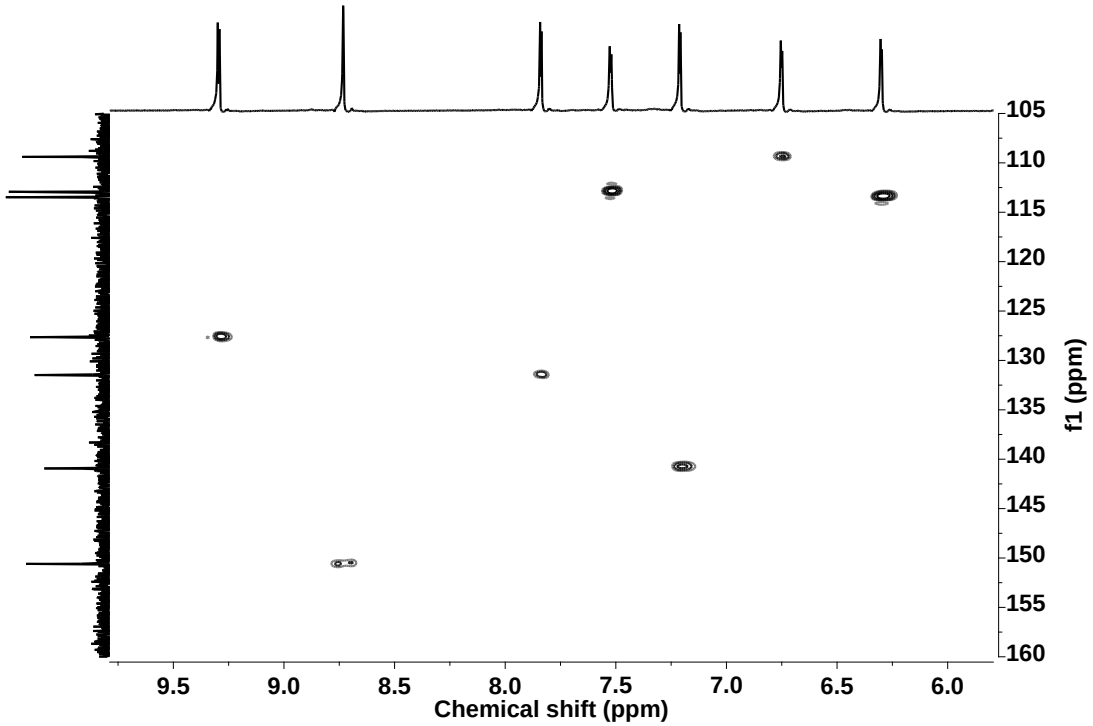
S9: ^{19}F-NMR spectrum of **5** in *Dimethyl Sulphoxide-d*$_6$ at 295K.



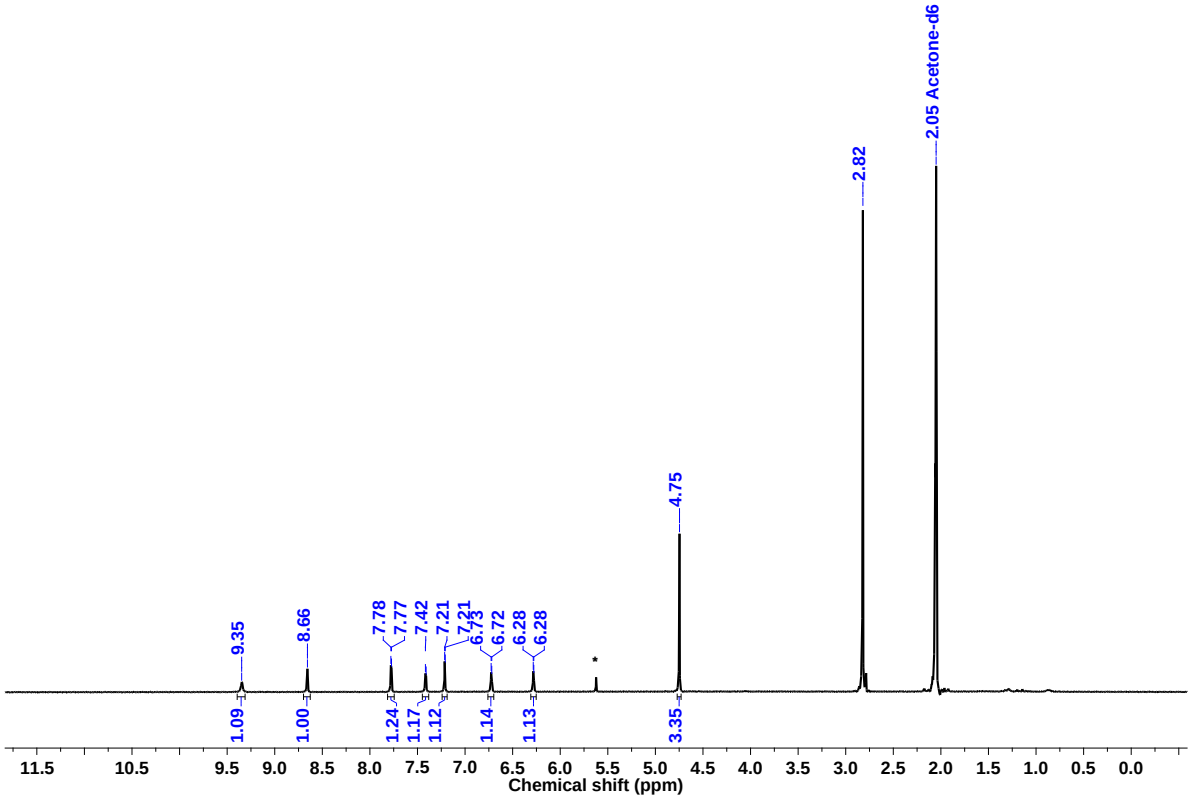
S10: ^{1}H-^{1}H COSY spectrum of **5** in *Dimethyl Sulphoxide-d*$_6$ at 295K.



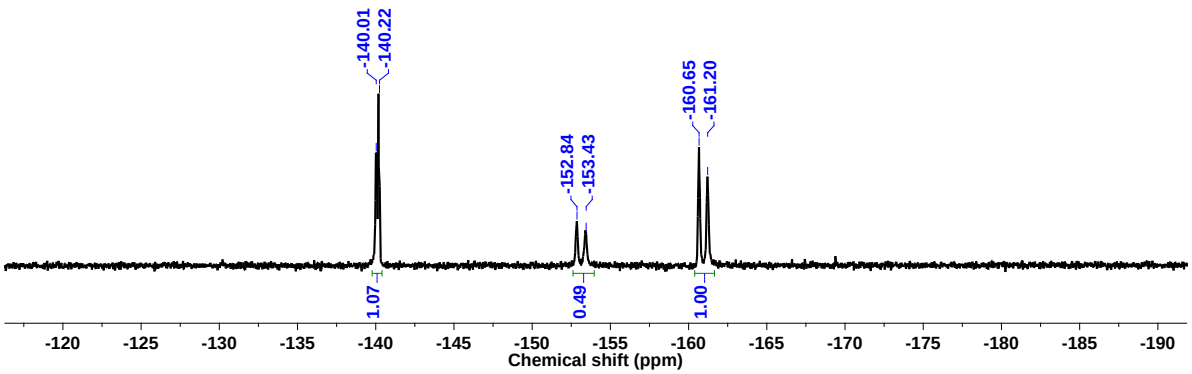
S11: (Top) DEPT-90 and (Bottom) ^{13}C-NMR spectrum of **5** in *Dimethyl Sulphoxide-d_6* at 295K.



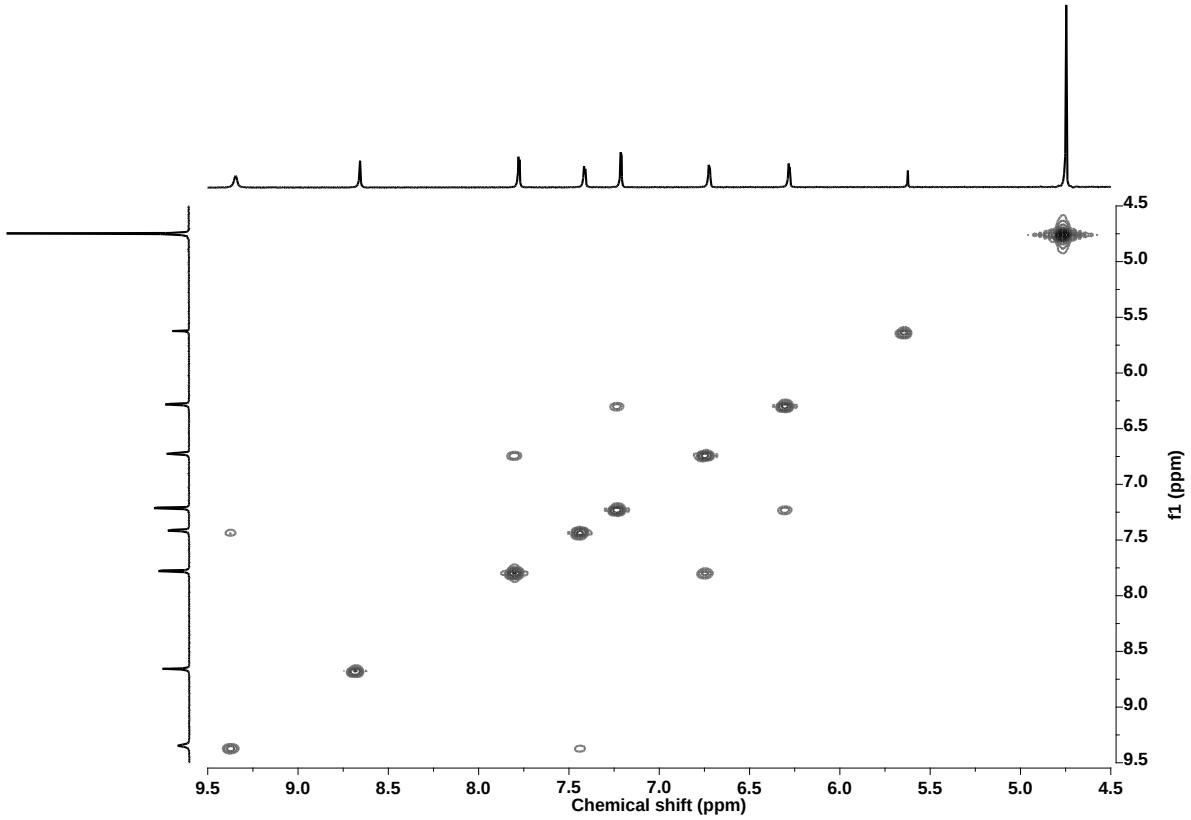
S12: HMBC spectrum of **5** in *Dimethyl Sulphoxide-d_6* at 295K.



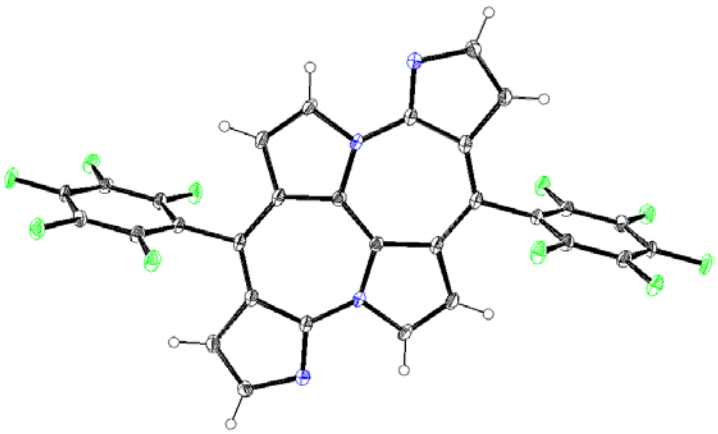
S13: ^{1}H-NMR spectrum of **Me-5** in *Acetone-d_6* at 295K.



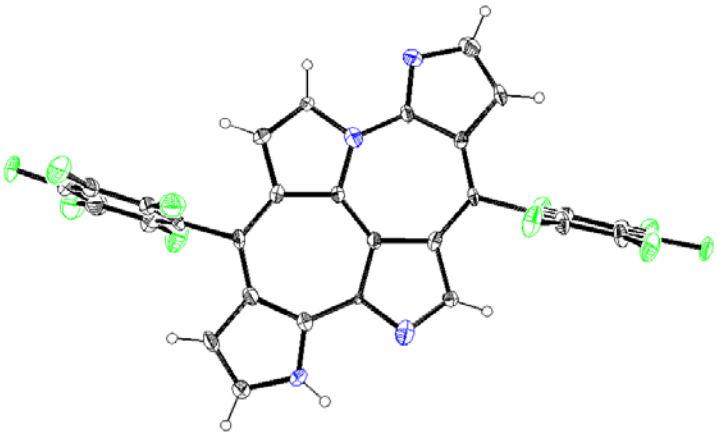
S14: ^{19}F-NMR spectrum of **Me-5** in *Acetone-d_6* at 295K.



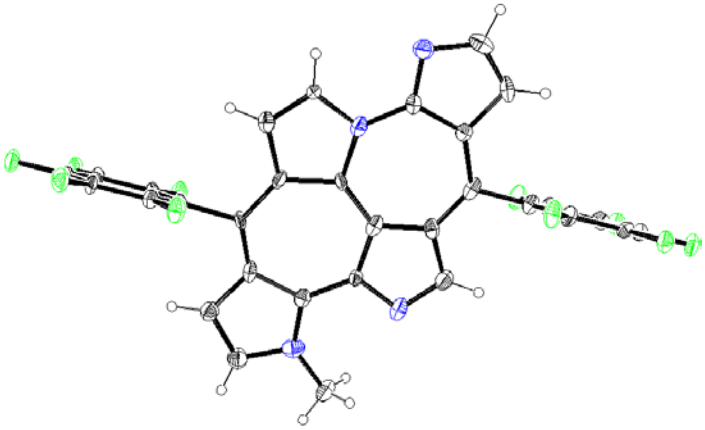
S15: ^{1}H-^{1}H COSY spectrum of **Me-5** in *Acetone-d_6* at 295K.



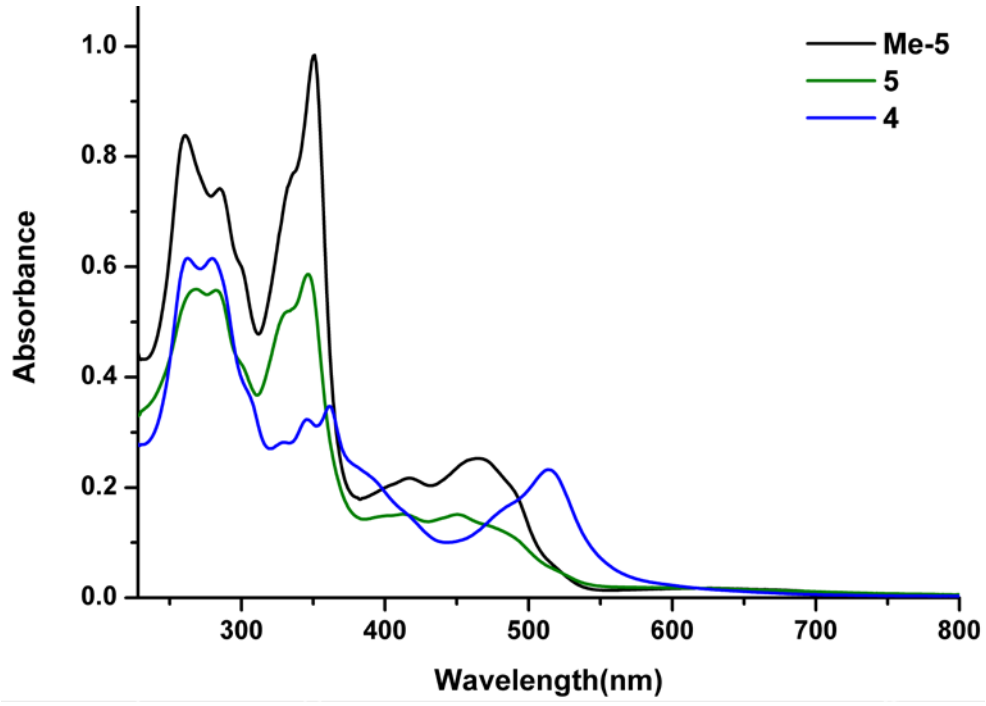
S16: ORTEP drawings of(top view) **4**. The thermal ellipsoids are scaled to the 50% probability level.



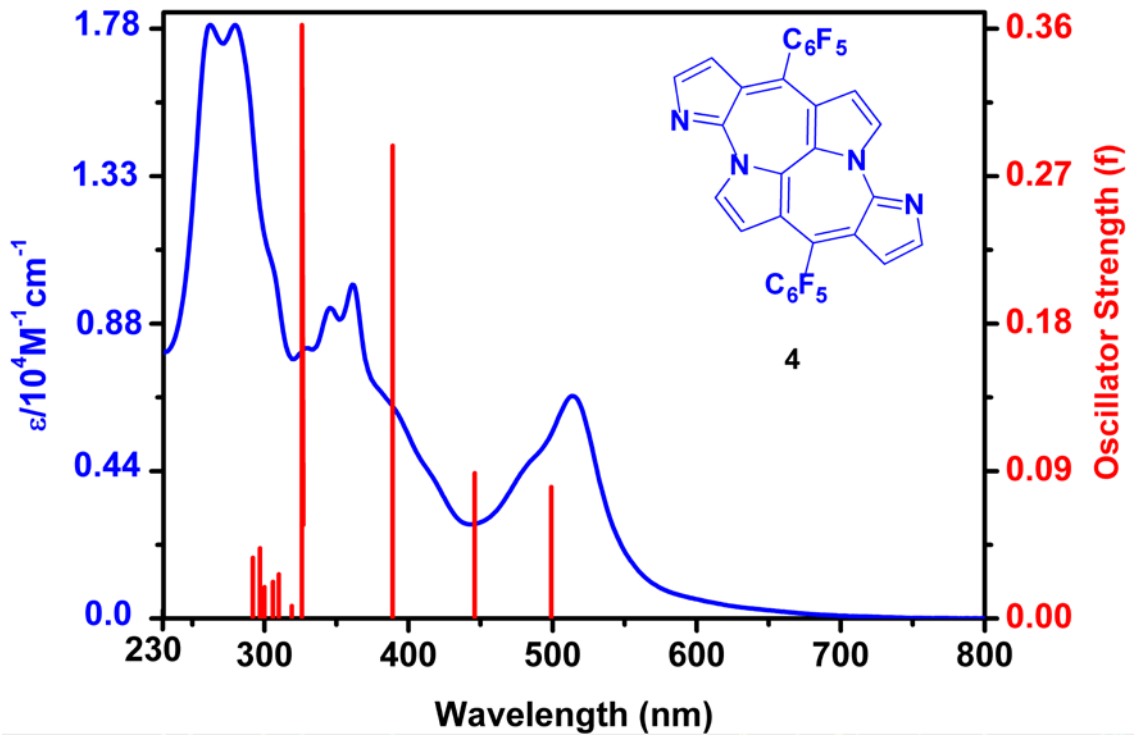
S17: ORTEP drawings of(top view) **5**. The thermal ellipsoids are scaled to the 50% probability level.



S18: ORTEP drawings of(top view) **Me-5**. The thermal ellipsoids are scaled to the 50% probability level.



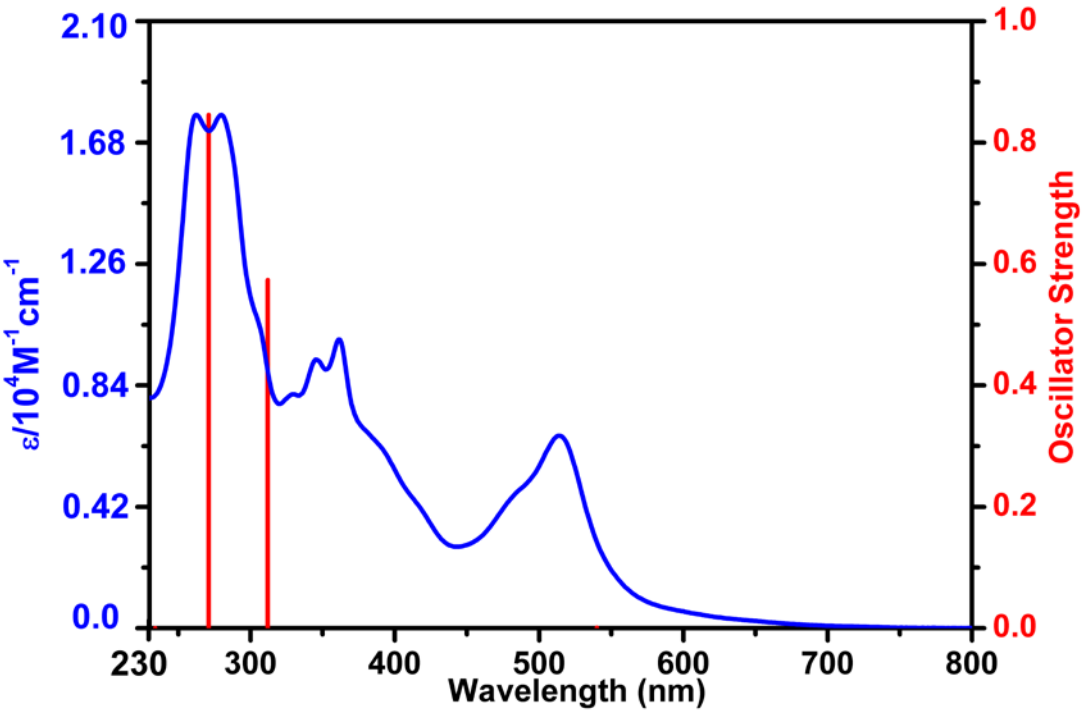
S19: UV-Visible spectrum of **4, 5** and **Me-5** at ~10^{-6} M in dichloromethane at 295K.



S20: The steady state absorption spectra (blue line) of **4** recorded in CH_2Cl_2 along with the theoretical vertical excitation energies (red bar) obtained from TD-DFT calculations carried out at the B3LYP/6-31G(d,p) level.

Energy (cm-1)	Wavelength (nm)	Osc. Strength (f)	Major contributions
30713.8048	325.5864933	0.3623	HOMO→L+2 (77%)
25679.25728	389.4193625	0.2886	H-2→LUMO (76%), HOMO→L+1 (15%)
22400.59088	446.4167956	0.0888	H-1→L+1 (91%)
20050.27504	498.7462756	0.0803	H-2→LUMO (19%), HOMO→L+1 (77%)
30616.21104	326.624349	0.0573	H-7→LUMO (29%), H-6→L+1 (37%), H-5→LUMO (11%)
33714.208	296.6108532	0.043	H-9→LUMO (15%), H-7→LUMO (20%), H-6→L+1 (52%)
34284.44592	291.677457	0.0371	H-10→L+1 (23%), H-9→LUMO (31%), H-8→L+1 (12%), H-7→LUMO (28%)
32249.49504	310.0823745	0.027	HOMO→L+3 (95%)
32656.00128	306.222428	0.0224	H-5→LUMO (37%), H-3→LUMO (19%), H-1→L+2 (27%)
33360.12816	299.7590403	0.0192	H-5→LUMO (16%), H-4→L+1 (52%), H-3→LUMO (28%)
31379.2168	318.6822687	0.0077	H-4→L+1 (44%), H-3→LUMO (43%)

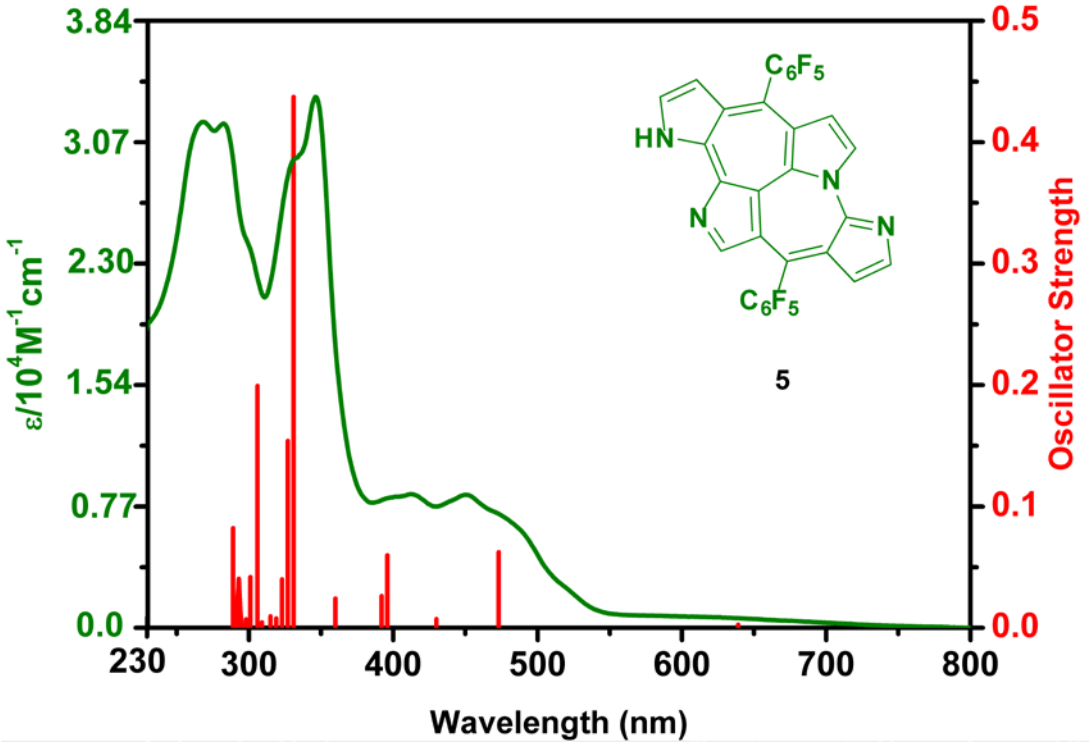
S21: Selected TD-DFT (B3LYP/6-31g (d, p)) calculated energies, oscillator strengths and compositions of the major electronic transitions of **4**.



S22: The steady state absorption spectra (blue line) of **4** recorded in CH_2Cl_2 and theoretical vertical excitation energies (red bar) for central fused seven membered bicyclic system **4** obtained from TD-DFT calculations carried out at the B3LYP/6-31G(d,p) level.

Energy (cm-1)	Wavelength (nm)	Osc. Strength (f)	Major contribs
36886.40848	271.1025663	0.8458	H-1L+1 (51%)
31950.26128	312.9864858	0.5737	H-1→LUMO (12%), H-1→L+1 (28%), HOMO→L+1 (25%)
18500.87328	540.5150259	0.0008	H-1→LUMO (63%), HOMO→L+1 (41%)
42612.17792	234.6746984	0.0001	HOMO→L+4 (98%)

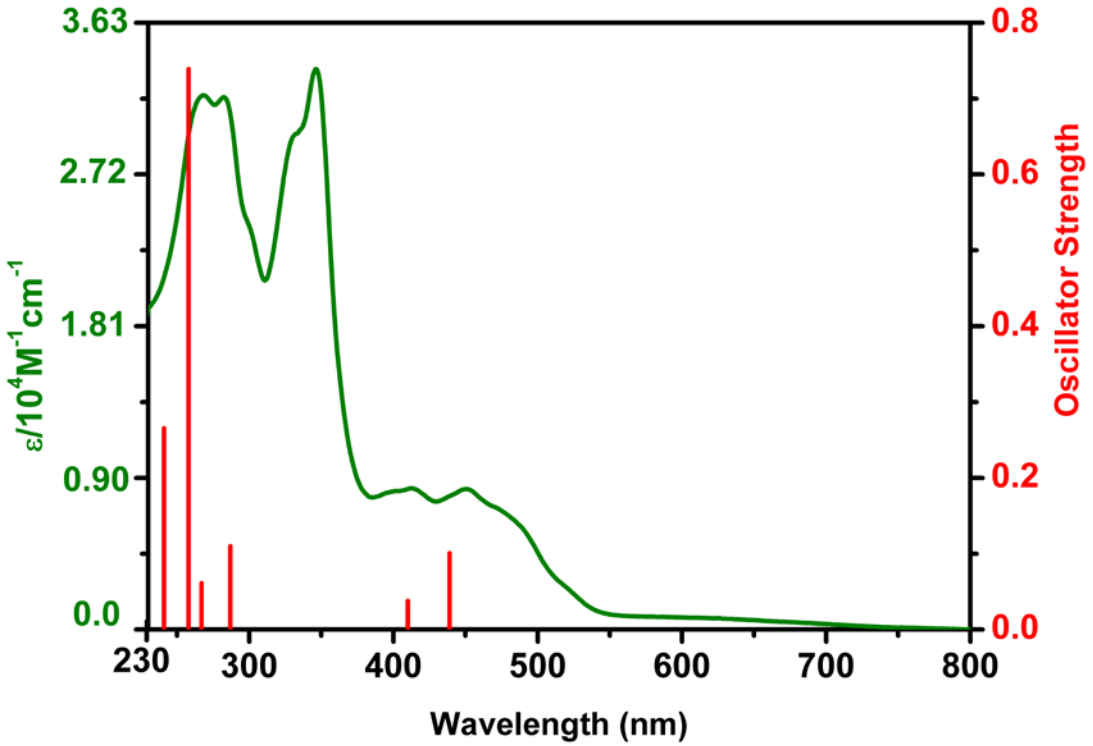
S23: Selected TD-DFT (B3LYP/6-31g (d, p)) calculated energies, oscillator strengths and compositions of the major electronic transitions for central fused seven membered bicyclic system **4**.



S24: The steady state absorption spectra (green line) of **5** recorded in CH_2Cl_2 along with the theoretical vertical excitation energies (red bar) obtained from TD-DFT calculations carried out at the B3LYP/6-31G(d,p) level.

Energy (cm-1)	Wavelength (nm)	Osc. Strength(f)	Major contributions
30200.83264	331.1166986	0.4373	H-4⟶LUMO (13%), HOMO⟶L+2 (35%), HOMO⟶L+3 (26%)
32660.84064	306.177055	0.1993	H-6⟶LUMO (23%), H-4⟶LUMO (29%), H-1⟶L+2 (11%), HOMO⟶L+2 (10%)
30570.23712	327.1155523	0.1541	H-4⟶LUMO (10%), HOMO⟶L+3 (71%)
34569.1616	289.2751671	0.0823	H-9⟶LUMO (25%), H-7⟶LUMO (23%), H-7⟶L+1 (13%)
21125.41952	473.3633806	0.0625	HOMO⟶L+1 (80%)
25276.78384	395.6199516	0.0599	H-1⟶L+1 (58%), HOMO⟶L+2 (23%)
33273.01968	300.5438068	0.0419	HOMO⟶L+5 (89%)
34069.90096	293.5142081	0.0404	H-9⟶LUMO (31%), H-8⟶LUMO (11%), H-7⟶LUMO (10%), H-4⟶L+1 (21%), H-3⟶L+1 (12%)
30950.12688	323.1004525	0.04	H-6⟶LUMO (29%), H-4⟶LUMO (26%), H-4⟶L+1 (14%)
25519.5584	391.8563105	0.0262	H-2⟶LUMO (78%)
27804.54288	359.6534582	0.0241	H-2⟶L+1 (89%)
34154.58976	292.7864182	0.0205	H-8⟶LUMO (51%), H-7⟶LUMO (23%)
33969.08096	294.3853563	0.0151	HOMO⟶L+6 (93%)
31777.65744	314.6865064	0.0095	H-3⟶LUMO (82%), H-3⟶L+1 (12%)
31309.04608	319.3965084	0.0077	HOMO⟶L+4 (96%)
23264.41664	429.8409951	0.0072	H-1⟶LUMO (78%), H-1⟶L+1 (13%)
33602.09616	297.6004816	0.007	H-9⟶LUMO (14%), H-6⟶LUMO (21%), H-4⟶L+1 (31%)

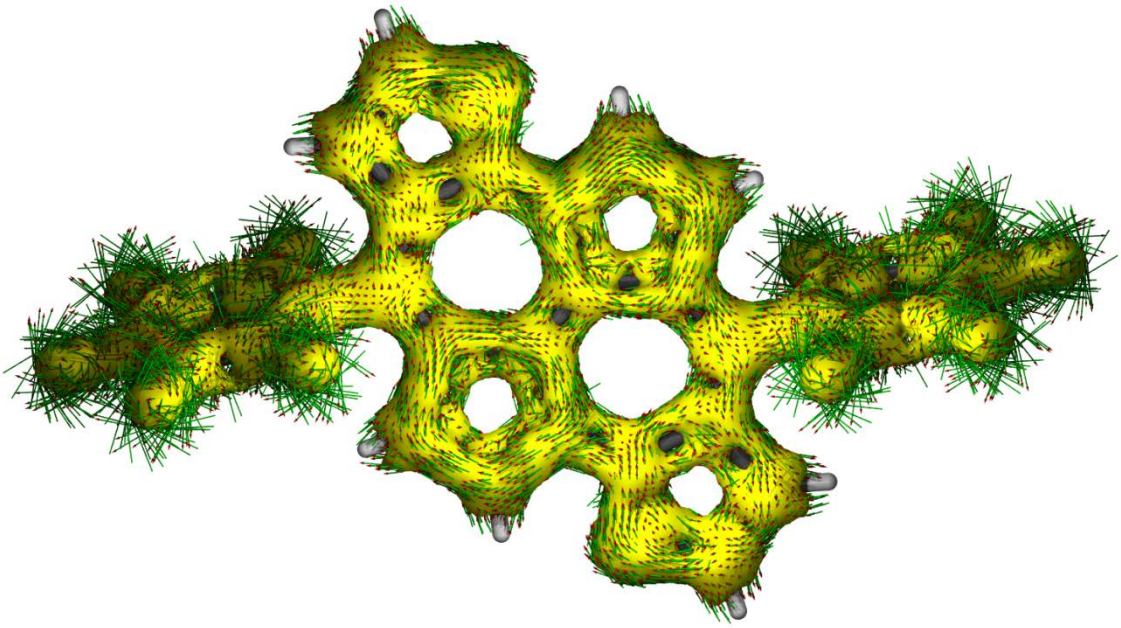
S25: Selected TD-DFT (B3LYP/6-31g (d, p)) calculated energies, oscillator strengths and compositions of the major electronic transitions of **5**.



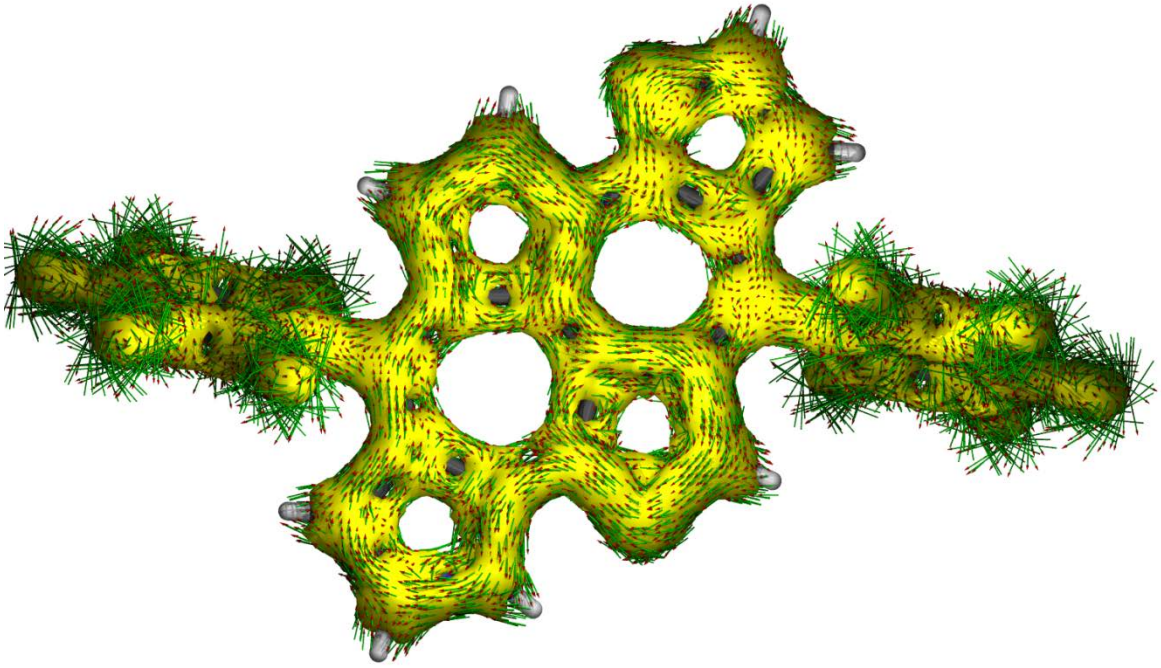
S26: The steady state absorption spectra (green line) of **5** recorded in CH_2Cl_2 and theoretical vertical excitation energies (red bar) for central fused seven membered bicyclic system **5** obtained from TD-DFT calculations carried out at the B3LYP/6-31G(d,p) level .

Energy (cm-1)	Wavelength (nm)	Osc. Strength (f)	Major contribs
20464.84688	488.642796	0.0015	H-1(A) →LUMO(A) (20%), HOMO(A) →L+1(A) (62%), HOMO(B) →L+1(B) (22%)
24406.5056	409.726823	0.0015	H-1(A) →L+1(A) (75%), HOMO(B) →L+2(B) (35%)
25920.41872	385.7962369	0.1212	H-1(A) →LUMO(A) (14%), HOMO(A) →L+1(A) (18%), H-1(B) →LUMO(B) (47%), HOMO(B) →L+1(B) (14%)
33028.632	302.7676108	0.003	H-2(A) →LUMO(A) (31%), H-1(B) →L+1(B) (59%)
34736.92608	287.8780919	0.0654	H-2(B) →LUMO(B) (26%), HOMO(B) →L+2(B) (44%)
35461.21696	281.9982183	0.6233	HOMO(A) →L+1(A) (13%), H-1(B) →LUMO(B) (35%)
36633.9552	272.9707984	0.003	HOMO(A) →L+2(A) (96%)
36868.66416	271.2330438	0.1205	H-1(A) →L+1(A) (11%), H-2(B) →LUMO(B) (49%)
38166.4192	262.0104325	0.0017	H-3(A) →LUMO(A) (29%), H-2(B) →L+1(B) (68%)
39934.39872	250.4106815	0.0224	H-3(B) →LUMO(B) (66%)
40590.132	246.3652988	0.0001	H-1(A) →L+2(A) (81%), HOMO(B) →L+3(B) (17%)
42883.98864	233.1872645	0.1404	H-2(A) →LUMO(A) (48%), H-1(B) →L+1(B) (21%)
44205.94048	226.2139407	0.0575	H-2(A) →L+1(A) (15%), HOMO(A) →L+6(A) (11%), H-5(B)→LUMO(B) (24%), H-1(B) →L+2(B) (14%)

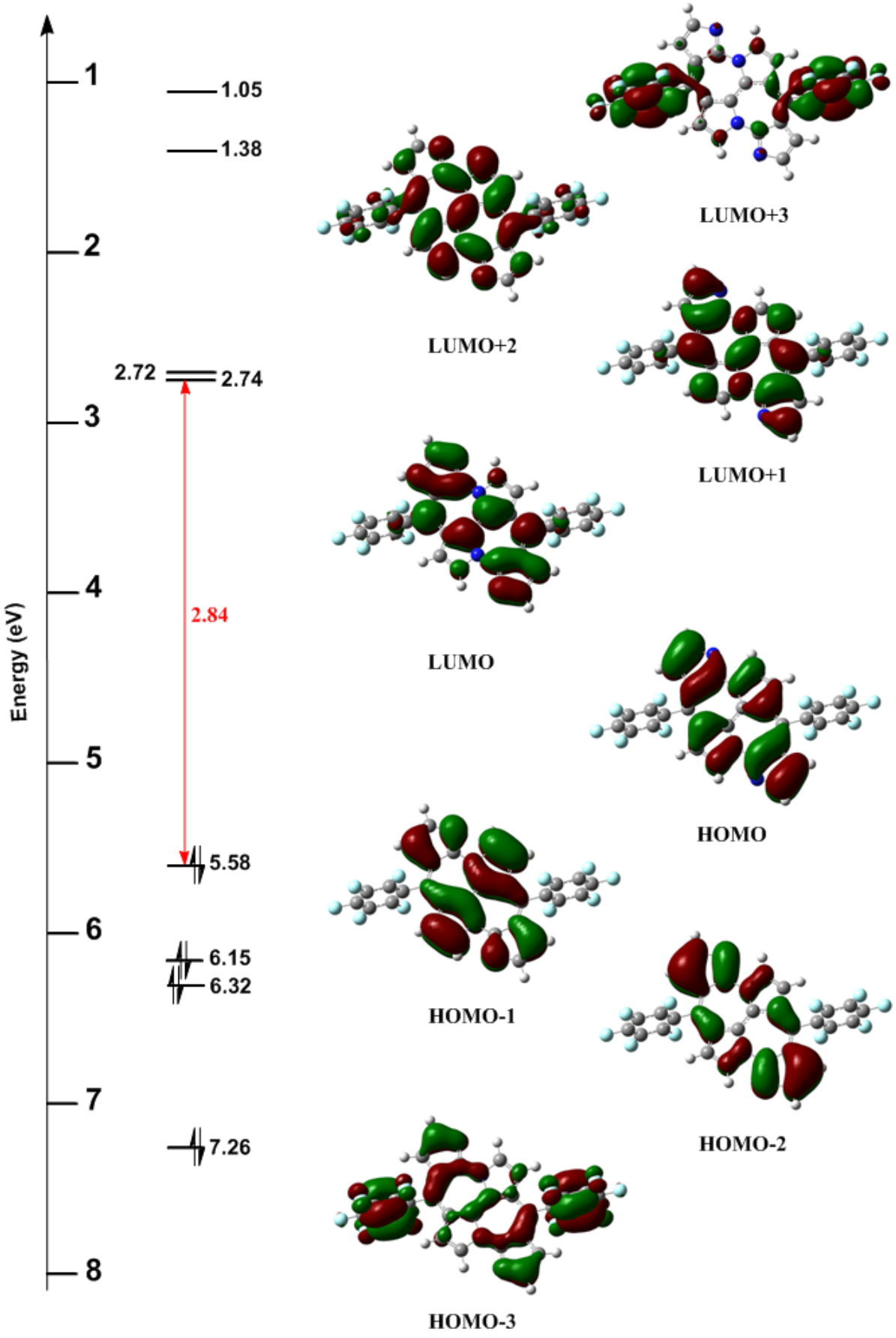
S27: Selected TD-DFT (B3LYP/6-31g (d, p)) calculated energies, oscillator strengths and compositions of the major electronic transitions for central fused seven membered bicyclic system **5**.



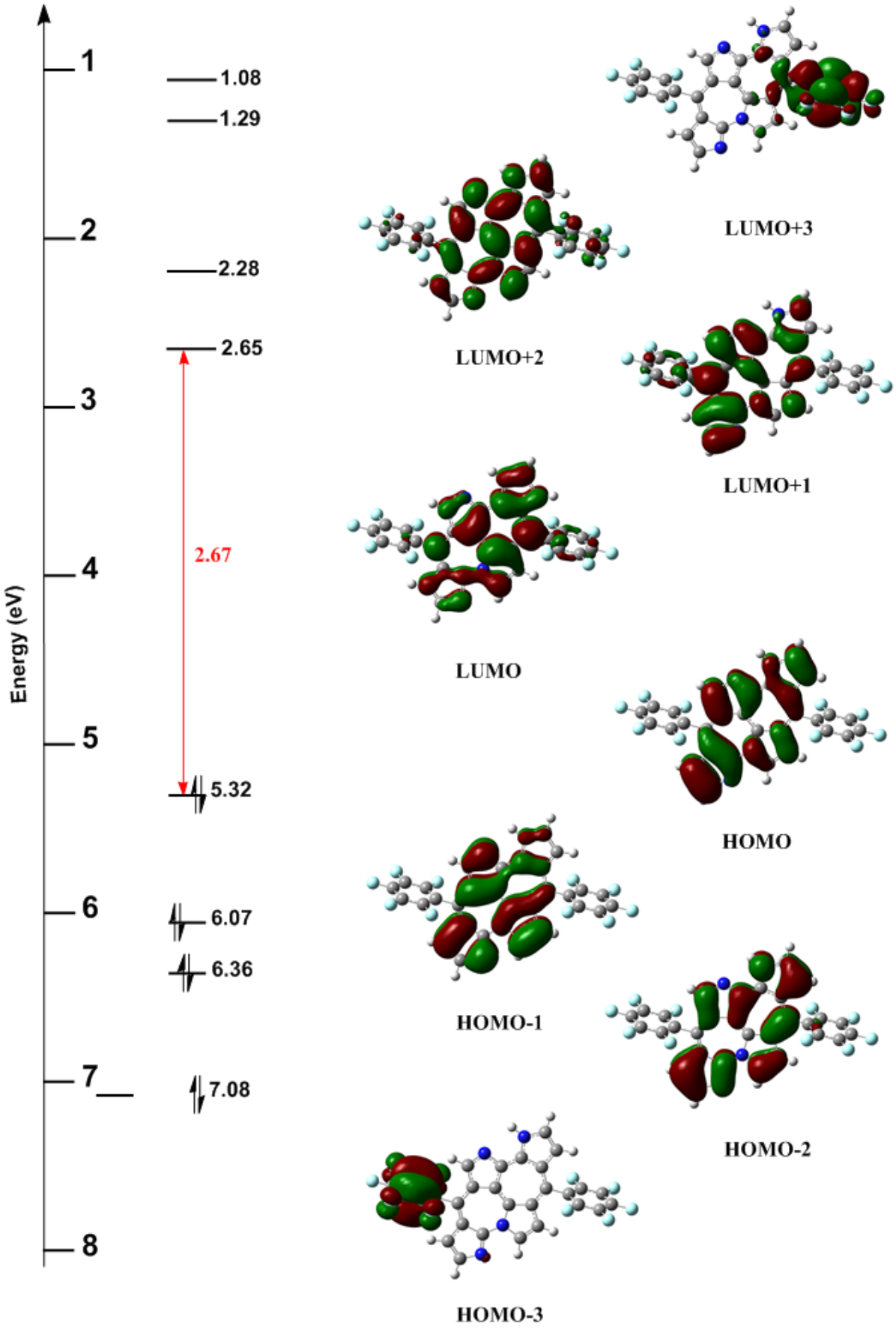
S28: AICD plot of **4** at an isosurface value of 0.05. The external magnetic field is applied orthogonal to the molecule plane.



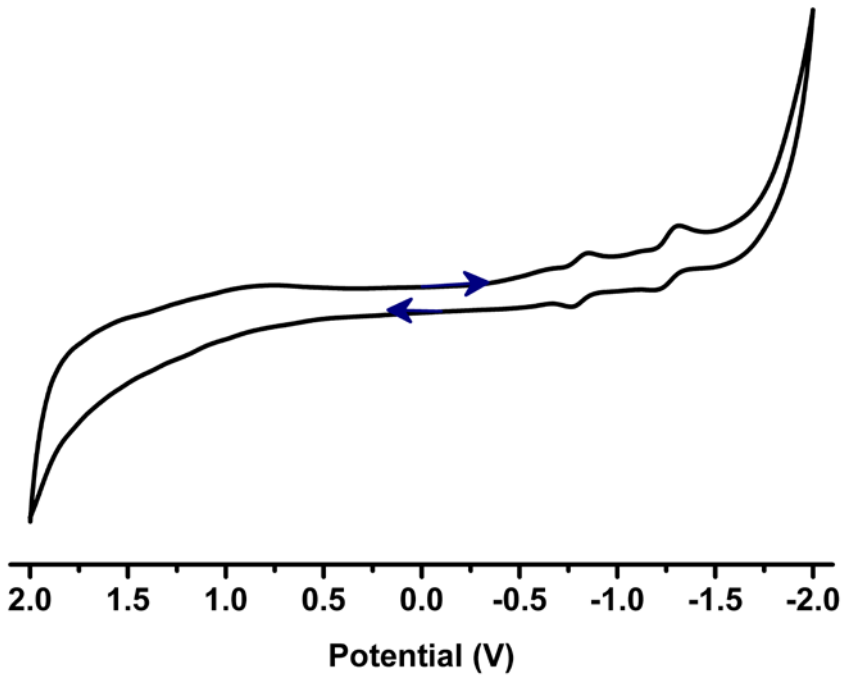
S29: AICD plot of **5** at an isosurface value of 0.05. The external magnetic field is applied orthogonal to the molecule plane.



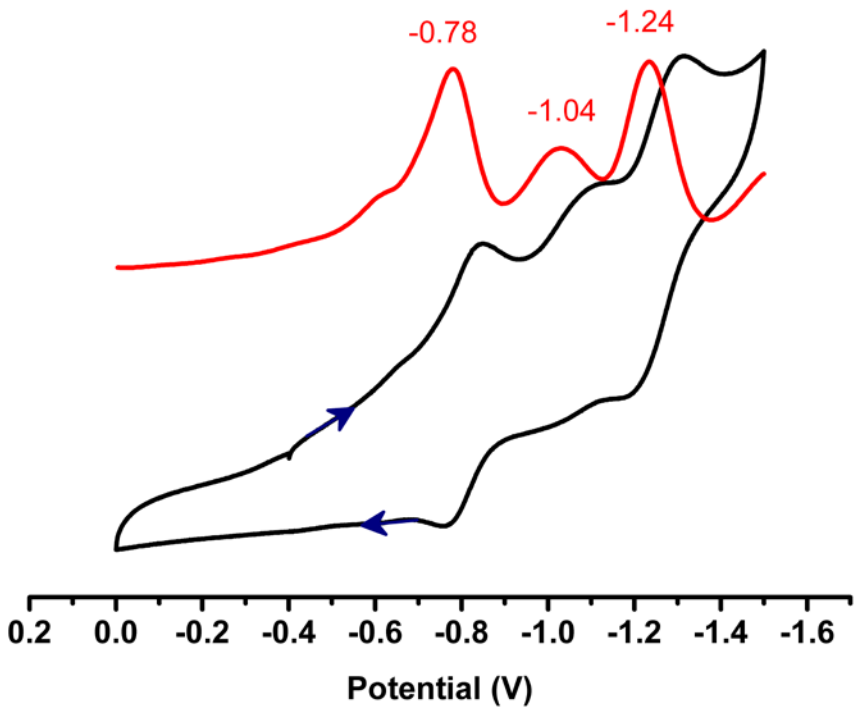
S30: Frontier MOs of **4** calculated at the B3LYP/6-31G(d,p) level.



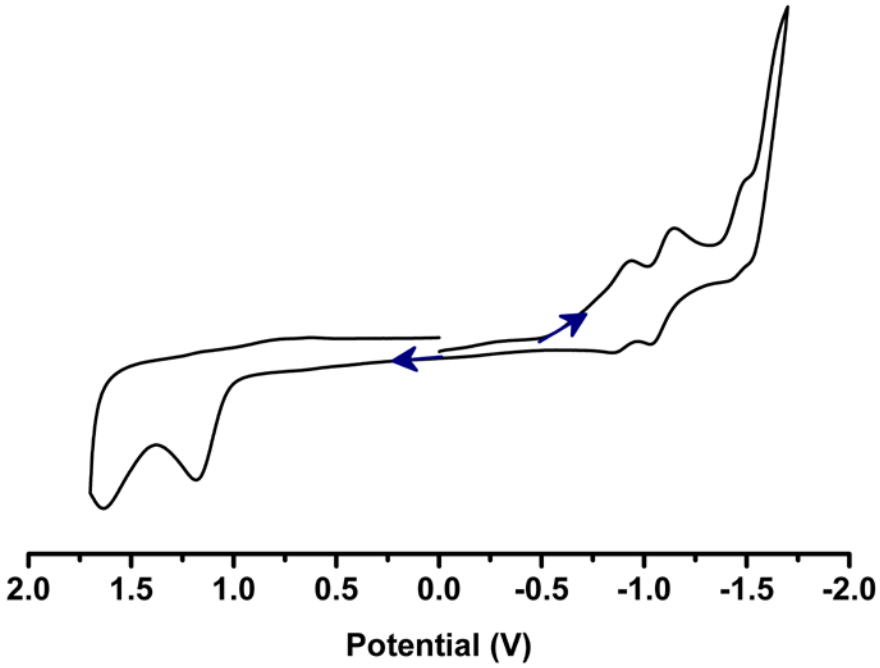
S31: Frontier MOs of **5** calculated at the B3LYP/6-31G(d,p) level.



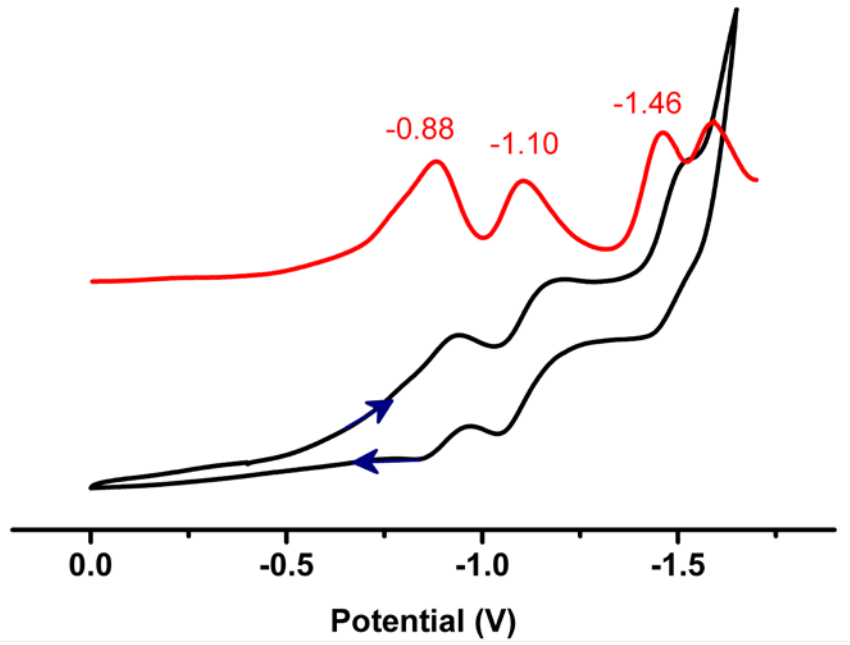
S32: Cyclic voltammogram of **4** were recorded in CH_2Cl_2 using TBAP as a supporting electrolyte.



S33: Cyclic voltammogram (black line) and differential pulse voltammogram (red line) of **4**.



S34: Cyclic voltammogram of **5** were recorded in CH_2Cl_2 using TBAP as a supporting electrolyte.



S35: Cyclic voltammogram (black line) and differential pulse voltammogram (red line) of **5**.

S36: Coordinates Table for optimized structure **4**

Sr.No.	Atom	X	Y	Z
1	F	8.309239	0.870351	-0.10525
2	F	4.510532	-1.0135	-2.14861
3	F	4.201537	0.844628	2.195586
4	F	6.831998	1.476199	2.108313
5	F	7.136521	-0.37487	-2.23097
6	N	-0.03957	-1.85781	0.345251
7	N	1.317301	-3.72693	0.688426
8	C	7.013311	0.556051	-0.06202
9	C	6.257869	0.866037	1.06692
10	C	4.906015	0.533255	1.099735
11	C	4.278124	-0.10675	0.02843
12	C	2.826487	-0.47911	0.088499
13	C	1.890591	0.56809	-0.10911
14	C	-0.44823	-0.53958	0.099549
15	C	5.059502	-0.40447	-1.09051
16	C	6.413464	-0.08063	-1.14612
17	C	2.275592	1.917484	-0.36823
18	H	3.287354	2.281545	-0.44993
19	C	-1.15331	-2.66831	0.505195
20	H	-0.99989	-3.71512	0.703687
21	C	2.5367	-1.80388	0.332575
22	C	1.230158	-2.43969	0.447463
23	C	2.6814	-4.00319	0.744685
24	H	3.006943	-5.01791	0.935436
25	C	3.455709	-2.89599	0.541819
26	H	4.533516	-2.83255	0.540466
27	F	-8.30924	-0.87035	0.105266
28	F	-4.51053	1.013504	2.148611
29	F	-4.20154	-0.84463	-2.19558
30	F	-6.832	-1.4762	-2.10831
31	F	-7.13652	0.374874	2.230979
32	N	0.039565	1.857805	-0.34526
33	N	-1.3173	3.726923	-0.68844
34	C	-7.01331	-0.55605	0.062029
35	C	-6.25787	-0.86604	-1.06691
36	C	-4.90602	-0.53326	-1.09973
37	C	-4.27812	0.106752	-0.02843
38	C	-2.82649	0.47911	-0.0885
39	C	-1.89059	-0.56809	0.109108
40	C	0.448227	0.539583	-0.09956
41	C	-5.0595	0.404467	1.090515
42	C	-6.41346	0.080631	1.14613
43	C	-2.27559	-1.91749	0.368227

44	H	-3.28735	-2.28155	0.449927
45	C	1.153311	2.668313	-0.5052
46	H	0.999888	3.71512	-0.70369
47	C	-2.5367	1.803878	-0.33258
48	C	-1.23016	2.439691	-0.44747
49	C	-2.6814	4.003191	-0.7447
50	H	-3.00694	5.017902	-0.93545
51	C	-3.45571	2.895991	-0.54183
52	H	-4.53352	2.832544	-0.54047

S37: Coordinates Table for optimized structure **5**

Sr.No.	Atom	X	Y	Z
1	F	-4.57163	-0.76353	-2.25958
2	F	-4.17918	0.590767	2.263799
3	F	-8.314	0.925217	0.040352
4	F	-7.18713	-0.08834	-2.22979
5	F	-6.79812	1.260953	2.284199
6	F	4.174106	-0.55408	2.277121
7	F	4.526863	0.705439	-2.27499
8	F	6.803643	-1.18197	2.302083
9	F	8.305238	-0.87382	0.045365
10	F	7.154418	0.071458	-2.24244
11	N	-1.34024	-3.81078	-0.0027
12	N	1.413804	3.789384	-0.04094
13	H	0.625205	4.421272	-0.04919
14	N	0.035522	-1.92476	-0.02506
15	C	-0.05595	1.885825	-0.03922
16	C	1.157499	-2.74571	-0.04056
17	H	1.008254	-3.81251	-0.05025
18	N	-1.13477	2.725122	-0.05677
19	C	-5.09528	-0.27078	-1.13041
20	C	-6.44513	0.073529	-1.12918
21	C	-7.02133	0.592359	0.027786
22	C	-2.2072	1.939337	-0.04787
23	H	-3.20354	2.364237	-0.06637
24	C	-4.29288	-0.10984	0.002277
25	C	-1.8979	0.55253	-0.02306
26	C	-2.54918	-1.8471	0.001974
27	C	-1.24667	-2.50182	-0.01174
28	C	-0.44645	0.499622	-0.02088
29	C	1.233682	2.437409	-0.03693
30	C	2.531122	1.836516	-0.01769
31	C	-3.47251	-2.95919	0.025362
32	H	-4.55006	-2.89131	0.050465

33	C	0.430591	-0.59164	-0.01871
34	C	-6.24595	0.764586	1.17198
35	C	1.893194	-0.60189	-0.02335
36	C	3.474305	2.930099	-0.00542
37	H	4.549503	2.847687	0.018054
38	C	-2.84409	-0.49651	-0.00634
39	C	4.886147	-0.39224	1.154655
40	C	2.278744	-1.98464	-0.04011
41	H	3.289072	-2.36084	-0.06074
42	C	2.812671	0.460517	-0.01421
43	C	-2.70633	-4.08872	0.020179
44	H	-3.03594	-5.11978	0.033416
45	C	2.7595	4.09267	-0.02027
46	H	3.096212	5.118699	-0.01752
47	C	-4.89824	0.41446	1.147326
48	C	4.266597	0.092408	-0.00075
49	C	5.063637	0.241158	-1.13911
50	C	7.007729	-0.56322	0.030091
51	C	6.239309	-0.72143	1.181318
52	C	6.419216	-0.07984	-1.13627

S38: Coordinates Table for optimized structure **Me-5**

Sr.No.	Atom	X	Y	Z
1	F	8.312488	0.813072	-0.03311
2	F	-8.26488	-1.05128	0.103598
3	F	6.81578	1.304121	2.195751
4	F	4.197136	0.630114	2.24516
5	F	-4.43287	0.637373	2.254668
6	F	-7.05498	-0.02334	2.323574
7	F	-6.82982	-1.41529	-2.18879
8	F	-4.20607	-0.76092	-2.26338
9	F	4.55252	-1.04098	-2.17294
10	F	7.167711	-0.36057	-2.21511
11	C	-6.23665	-0.91349	-1.10089
12	N	1.168627	2.580286	-0.34218
13	N	-0.01747	-2.03169	0.241907
14	N	1.354103	-3.90832	0.477173
15	C	7.020426	0.47762	-0.00987
16	C	6.255045	0.728897	1.126476
17	C	4.908002	0.3756	1.138575
18	C	4.294088	-0.22896	0.038997
19	C	2.845868	-0.61937	0.073536
20	C	1.897992	0.420801	-0.06253

21	C	0.445387	0.387845	-0.05652
22	C	-0.41729	-0.70662	0.077637
23	C	-1.87415	-0.72617	0.083321
24	C	-2.78481	0.329514	-0.04914
25	C	-4.23863	-0.04369	-0.00606
26	C	-4.8867	-0.57052	-1.12583
27	C	-6.97067	-0.72744	0.06846
28	C	0.06424	1.779895	-0.23334
29	C	2.226715	1.78712	-0.24279
30	H	3.228453	2.194702	-0.30658
31	C	-1.22889	2.344201	-0.29943
32	C	-2.51301	1.695457	-0.21971
33	C	-3.5038	2.728511	-0.35351
34	H	-4.57387	2.596906	-0.3458
35	C	-2.83969	3.905442	-0.49921
36	H	-3.22157	4.907918	-0.62629
37	N	-1.47329	3.691315	-0.46837
38	C	-0.51415	4.788038	-0.60217
39	H	0.127733	4.85117	0.275839
40	H	-1.08853	5.70999	-0.71209
41	H	0.125277	4.640628	-1.47181
42	C	1.260989	-2.60969	0.312332
43	C	2.721251	-4.18212	0.520845
44	H	3.051148	-5.20476	0.652601
45	C	3.487437	-3.06077	0.385475
46	H	4.565156	-2.99046	0.390912
47	C	2.561634	-1.96013	0.238179
48	C	-1.13783	-2.84872	0.350146
49	H	-0.98468	-3.9065	0.484424
50	C	-2.26084	-2.09687	0.259447
51	H	-3.27114	-2.4693	0.316868
52	C	-5.00024	0.131986	1.151658
53	C	-6.35183	-0.20234	1.200676
54	C	5.085922	-0.46848	-1.08656
55	C	6.435042	-0.1226	-1.12197

S39: Coordinates Table for optimized structure of central fused seven membered bicyclic system **4**

Sr. No.	Atom	X	Y	Z
1	N	1.160627	-1.472125	0.000538
2	C	2.540288	1.256408	0.000096
3	C	1.157669	1.553328	0.000359
4	C	-0.018578	-0.7681	-0.000072
5	C	3.140658	0.009003	-0.000225

6	C	2.503643	-1.223454	-0.00023
7	N	-1.160626	1.472125	-0.000567
8	C	-2.540289	-1.256408	-0.000061
9	C	-1.15767	-1.553328	-0.000333
10	C	0.018579	0.768099	0.000071
11	C	-3.140658	-0.009002	0.000229
12	C	-2.503643	1.223454	0.0002
13	H	-0.947658	-2.624258	-0.000617
14	H	-3.197652	-2.120454	-0.000165
15	H	-4.225957	0.032975	0.000604
16	H	-3.090255	2.133612	0.000019
17	H	-0.969435	2.465857	-0.000925
18	H	0.947656	2.624258	0.000655
19	H	3.197651	2.120455	0.000226
20	H	4.225957	-0.032974	-0.000598
21	H	3.090256	-2.133611	-0.000077
22	H	0.969437	-2.465857	0.000879

S40: Coordinates Table for optimized structure of central fused seven membered bicyclic system **5**

Sr. No.	Atom	X	Y	Z
1	N	1.609392	-1.334423	-0.577677
2	C	-0.787145	1.561022	-0.03841
3	C	1.642189	1.514711	-0.383691
4	C	3.263863	-0.071697	0.658758
5	C	2.662191	-1.234956	0.367065
6	C	0.398834	0.735713	-0.239514
7	C	-2.103269	1.280645	0.105534
8	C	0.389093	-0.637549	-0.30435
9	C	-0.767687	-1.505447	-0.160859
10	C	2.881355	1.191182	0.044632
11	C	-2.087762	-1.251838	0.005847
12	H	-0.515161	-2.56407	-0.208895
13	H	-2.723493	-2.133823	0.06321
14	H	-2.75327	2.145679	0.224523
15	H	-0.553931	2.623608	-0.012459
16	H	1.504018	2.51476	-0.791824
17	H	3.66085	1.945697	-0.047161
18	H	4.085396	-0.077179	1.369457
19	H	2.980556	-2.164257	0.83824
20	H	1.432177	-2.293816	-0.843078
21	C	-2.815462	0.005621	0.130314
22	C	-4.164249	-0.019929	0.277171
23	H	-4.714889	-0.95427	0.296971
24	H	-4.739694	0.893754	0.379779