Supporting information for

Gallium(III)Corrole-BODIPY Hybrid: Novel Photophysical Properties and First Observation of B-F---F interactions

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Experimental section:

Instruments and experimental methods: ^{1}H, ^{13}C, ^{19}F and ^{11}B NMR spectra were recorded on Bruker 400 and 500 MHz using $CDCl_3$ as a solvent. Chemical shifts were given in parts per million relative to residual $CHCl_3$ (7.260 ppm). Two-dimensional (2D) NMR experiments were performed on a Bruker 500 MHz instrument. UV-Vis absorption experiments were performed on an Agilent Cary-100 with 1cm path length quartz cuvette and fluorescence emission spectra were recorded on a Horiba Fluorolog spectrophotometer. Matrix assisted LASER desorption/ionization (MALDI) were recorded on a Bruker ultra flextreme mass spectrometer. Cyclic voltammograms were carried out using a three-electrode system consisting of a Pt disk as working electrode, Ag/Ag^{+} reference electrode and a Pt-wire as counter electrode on a CH-Instrument potentiostat. Tetrabutylammonium hexafluorophosphate (TBAPF) was used as supporting electrolyte (0.1 M).

Crystal growth and X-ray crystal structures determination: Single crystal of **4M.Py.Hex** was obtained by slow diffusion of hexane into dichloromethane solution of **4** in presence of small amount of pyridine at 4°C. Single crystal of **4O.Py.Tol** was obtained by slow diffusion of hexane into dichloromethane/toluene(1:1,*v/v*) solution of **4** in presence of small amount of pyridine at 4°C. X-ray diffraction measurements were carried out at 120 K (**4M.Py.Hex**) and 100 K (**4O.Py.Tol**), on Bruker APEX II diffractometer equipped with a graphite monochromator and Mo Kα (λ = 0.71073 Å) radiation. Data collections were performed using ϕ and ω scans. The structures were solved using direct methods followed by full matrix least square refinements against F^2 (all data HKLF 4 format) using SHELXTL (Sheldrick, G. M. (2013). SHELXT, Universität Göttingen, Germany). Multiscan absorption correction and scaling was performed with SADABS[1]. All refinements were carried out using SHELXL 2014.1,[2] PLATON[3] program and WinGX v2014.1.[4]

Synthesis of compound 2: Compound **1** (200 mg, 0.25 mmol) and $GaCl_3$ (441 mg, 2.5 mmol) was dissolved in 50 ml of dry pyridine under Argon, refluxed for 2 hrs and allowed to cooled at room temperature. Solvent was evaporated to dryness under reduced pressure and subjected to column chromatography with silica gel (100-200 mesh) using hexane/CH_2Cl_2/pyridine (80:20:0.5, *v/v/v*) as eluent. Precipitation with hexane and few drops of CH_2Cl_2 gave desired product. Yield = 86.6 % (205 mg, 0.22 mmol), purple coloured crystalline solid. ^{1}H NMR (400 MHz, $CDCl_3$, 298 K): δ 9.2 (d, $^{3}J_{H-H}$ = 4.0 Hz, 2H), 8.87 (d, $^{3}J_{H-H}$ = 4.5 Hz, 2H), 8.80 (d, $^{3}J_{H-H}$, *J* = 4.0 Hz, 2H), 8.66 (d, $^{3}J_{H-H}$ = 4.5 Hz, 2H), 6.53 (m, 1H), 5.96 – 5.76 (m, 2H), 3.50 (m, 2H). ^{19}F NMR (376 MHz, $CDCl_3$): δ -137.61 – -137.92 (m, 6F), -153.71 (t, $^{3}J_{F-F}$ = 20.9 Hz, 2F), -153.90 (t, $^{3}J_{F-F}$ = 20.9 Hz, 1F), -162.19 – -162.48 (m, 4F), -162.57 (m, 2F). MS (MALDI-TOF, without matrix): Calculated for $C_{37}H_8F_{15}GaN_4$ [(M-Py)$^{+}$]: 861.9765, Observed: m/z 862.196. Anal. calc. for $C_{42}H_{13}F_{15}GaN_5$ (Fw: 941.019) C, 53.53; H, 1.39; N, 7.43. Found: C, 53.49; H, 1.43; N, 7.46

Synthesis of 3a and 3b: Freshly distilled $POCl_3$ (2.5 ml) was slowly added to DMF (3.5 ml), cooled in an ice bath under argon atmosphere and stirred for 10 minute. After warming to room temperature, the Vilsmeier complex was stirred for 30 minutes and diluted by adding 10 ml of dry CH_2Cl_2. This solution was added dropwise to ice cold CH_2Cl_2 solution of **2** (200 mg, 0.21 mmol) in 10 ml. During addition, the solution color turned from red to green. After 5-6 minutes ice was removed and stirred for another 10 minutes. This reaction mixture was added dropwise into a saturated aqueous solution of K_2CO_3 (600 ml) cooled in an ice bath with continuous stirring. After warming to room temperature, the reaction mixture was further stirred overnight and extracted with CH_2Cl_2. The organic layers were combined, washed with water, dried over anhydrous $NaSO_4$ and the solvent was removed under reduced pressure. The crude product was purified by silica gel column chromatography (100-200 mesh) using hexane/CH_2Cl_2/pyridine (80:20:0.5, *v/v/v*) as an eluent, and recrystallization with hexane/CH_2Cl_2 and few drops of pyridine gave **3a**. Yield = 9.8%, (22 mg, 0.02 mmol), green solid. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K): δ 10.54 (s, 1H), 9.68 (s, 1H), 9.13 (d, $^{3}J_{H-H}$ = 4.1 Hz, 1H), 8.78 (d, $^{3}J_{H-H}$ = 4.5 Hz, 1H), 8.75 (d, $^{3}J_{H-H}$ = 4.1 Hz, 1H), 8.70 (d, $^{3}J_{H-H}$ = 4.7 Hz, 1H), 8.55 (d, $^{3}J_{H-H}$ = 4.5 Hz, 1H), 8.51 (d, $^{3}J_{H-H}$ = 4.4 Hz, 1H), 6.79 (t, $^{3}J_{H-H}$ = 7.6 Hz, 1H), 6.02 (t, $^{3}J_{H-H}$ = 6.7 Hz, 2H), 3.33 (s, 2H). ^{19}F NMR (376 MHz, $CDCl_3$): δ -137.36 – -138.07 (m, 4H), -138.57 (d, $^{3}J_{H-H}$ = 7.8 Hz, 1H), -138.63 ($^{3}J_{H-H}$, *J* = 7.9 Hz, 1H), -152.94 (m, 3H), -161.73 (m, 2 H), -161.97 (m, 2H), -162.28 (m, *2*H). MS (MALDI-TOF, without matrix): Calculated for $C_{38}H_8F_{15}GaN_4O$ [(M-Py)$^{+}$]:

889.9714, Observed: m/z 890.201. Anal. calc. for $C_{43}H_{13}F_{15}GaN_5O$ (Fw: 969.014) C, 53.23; H, 1.35; N, 7.22. Found: C, 53.17; H, 1.45; N, 7.26

Further, elution with hexane/CH_2Cl_2/pyridine (60:40:1, *v/v/v*) as eluent followed by recrystallization with hexane/CH_2Cl_2 and few drops of pyridine gave **3b**. Yield = 62% (142 mg, 0.13 mmol), green solid. ^{1}H NMR (500 MHz, $CDCl_3$): δ 11.15 (s, 1H), 10.59 (s, 1H), 10.04 (s, 1H), 9.03 (s, 1H), 8.70 (d, $^3J_{H-H}$ = 4.6 Hz, 1H), 8.63 (d, $^3J_{H-H}$ = 4.7 Hz, 1H), 8.41 (t, *J* = 4.6 Hz, 2H), 7.22 (tt, $^3J_{H-H}$ = 7.7 Hz, $^4J_{H-H}$ = 1.5 Hz, 2H), 6.60 (m, 4H), 5.54 (m, 4H). ^{19}F NMR (471 MHz, $CDCl_3$): δ -137.71 (m, 4F), -139.17 (d, $^3J_{F-F}$ = 7.8 Hz, 1F), -139.22 (d, $^3J_{F-F}$ = 7.9 Hz, 1H), -151.82 (t, $^3J_{F-F}$ = 20.8 Hz, 1F), -152.41 (t, $^3J_{F-F}$ = 20.8 Hz, 1F), -152.75 (t, $^3J_{F-F}$ = 20.8 Hz,1F), -161.14 (td, $^3J_{F-F}$ = 22.9 Hz, $^4J_{F-F}$ = 7.4 Hz, 2F), -161.53 (td, $^3J_{F-F}$ = 23.7Hz, $^4J_{F-F}$ =8.1 Hz, 2F), -162.39 (td, $^3J_{F-F}$ = 24.0 Hz, $^4J_{F-F}$ = 8.0 Hz, 2F). MS (MALDI-TOF, without matrix): Calculated for $C_{39}H_8F_{15}GaN_4O_2$ [(M-2Py)$^+$]: 917.9664, Observed: m/z 918.204. Anal. calc. for $C_{49}H_{18}F_{15}GaN_6O_2$ (Fw: 1076.051) C, 54.62; H, 1.68; N, 7.80. Found: C, 54.54; H, 1.77; N, 7.82

Synthesis of compound 4*:* **3b** (100 mg, 0.093 mmol) and 2,4-dimethylpyrrole (40.2 µl, 0.39 mmol) were dissolved in 50 ml of dry CH_2Cl_2 and degassed with Argon for 30 minutes. Calatytic amount of TFA (10 µl) was added, and the solution was stirred for 4 hrs at room temperature under argon. The weak red colored fluorescence of the solution gradually intensifies as the reaction progress. When thin layer chromatography (TLC) shows complete consumption of aldehyde, dichloromethane (5 ml) solution of 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ, 22 mg, 0.093 mmol) was added, and stirring was continued for 30 minutes. Then two drop of N,N-diisopyropylethylamine (DIPEA) was added, stirred for another 5 minutes, and the solvent was concentrated (~20 ml) under reduced pressure. This crude product was partially purified by passing it through silica gel column (60-120 mesh) using hexane/CH_2Cl_2/pyridine (50:50:0.02, *v/v/v*) as eluent, and all collected solvent fractions were evaporated to dryness to afford dark greenish coloured sticky product.

The partially purified product was dissolved in 50 ml of dry CH_2Cl_2 under Argon atmosphere and 1 ml of DIPEA was added slowly to it and stirred for 30 minutes at room temperature. Then, 1 ml of $BF_3.OEt_2$ was added to the ice cold reaction mixture and stirred for 5 minutes. Ice bath was removed and stirred for another 2 hrs at room temperature. The reaction mixture was concentrated under reduced pressure and filtered through silica gel (100-200 mesh) column chromatography using CH_2Cl_2/pyridine (100:0.5, v/v) as eluent. Three subsequent silica gel (100-200 mesh) column chromatography using hexane/CH_2Cl_2/pyridine (70:30:0.5, v/v/v) as eluent was performed and recrystallization with hexane/CH_2Cl_2 with small amount of pyridine afforded **4**. Yield = 9.2% (13 mg, 0.0085 mmol), dark greenish solid. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K): δ 8.92 (d, $^3J_{H-H}$ = 4.5 Hz, 1H), 8.75 (s, 1H), 8.74 (s, 1H), 8.71 (s, 1H), 8.68 (d, $^3J_{H-H}$ = 4.6 Hz, 1H), 8.62 (d, $^3J_{H-H}$ = 4.6 Hz, 1H), 6.93 (m, 1H), 6.09 (m, 2H), 5.90 (s, 4H), 3.58 (d, $^3J_{H-H}$ = 4.3 Hz, 2H), 2.66 (s, 6H), 2.60 (s, 6H), 0.64 (s, 6H), 0.59 (s, 6H). ^{11}B NMR (160 MHz, $CDCl_3$): δ 0.90 (m, -BF_2, 2B). ^{19}F NMR (471 MHz, $CDCl_3$): δ -137.58 (d, $^3J_{F-F}$ = 20.6 Hz, 2F), -137.70 (dd, $^3J_{F-F}$ = 24.1 Hz, $^4J_{F-F}$ = 7.6 Hz, 2F), -138.26 (dd, $^3J_{F-F}$ = 23.8 Hz, $^4J_{F-F}$ =7.2 Hz, 2F), -145.38 – -146.61 (m, 3F), -147.20 (m, 1F), -149.90 (q, $^3J_{F-F}$ = 19.8 Hz, 1F), -152.48 (t, $^3J_{F-F}$ = 20.8 Hz, 1F), -152.91 (t, *J* = 20.9 Hz, 1F), -161.41 (td, $^3J_{F-F}$ = 23.9 Hz, $^4J_{F-F}$ 8.0 Hz, 2F), -161.91 (td, $^3J_{F-F}$ = 23.9 Hz, $^3J_{F-F}$ = 7.9 Hz, 2F), -163.99 – -164.49 (m, 2F). MS (MALDI-TOF, without matrix): Calculated for $C_{63}H_{34}F_{18}B_2GaN_8$ [(M-Py)$^+$]: 1335.2061, Observed: m/z 1335.465. Anal. calc. for $C_{68}H_{39}B_2F_{19}GaN_9$ (Fw: 1433.247) C, 56.94; H, 2.74; N, 8.79. Found: C, 56.82; H, 2.81; N, 8.85

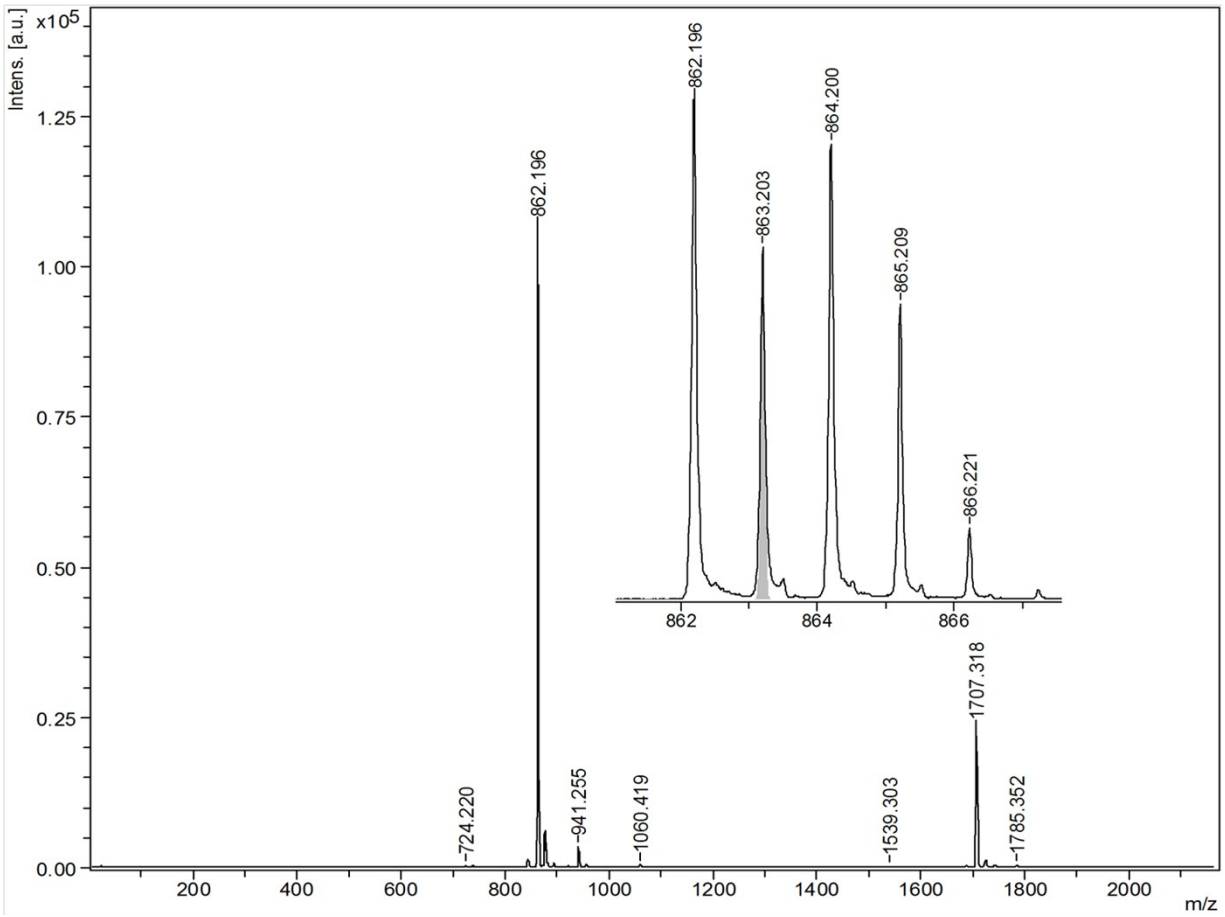

Fig. S1: Mass spectra of compound **2.** Inset: represent isotopic pattern of molecular ion peak.

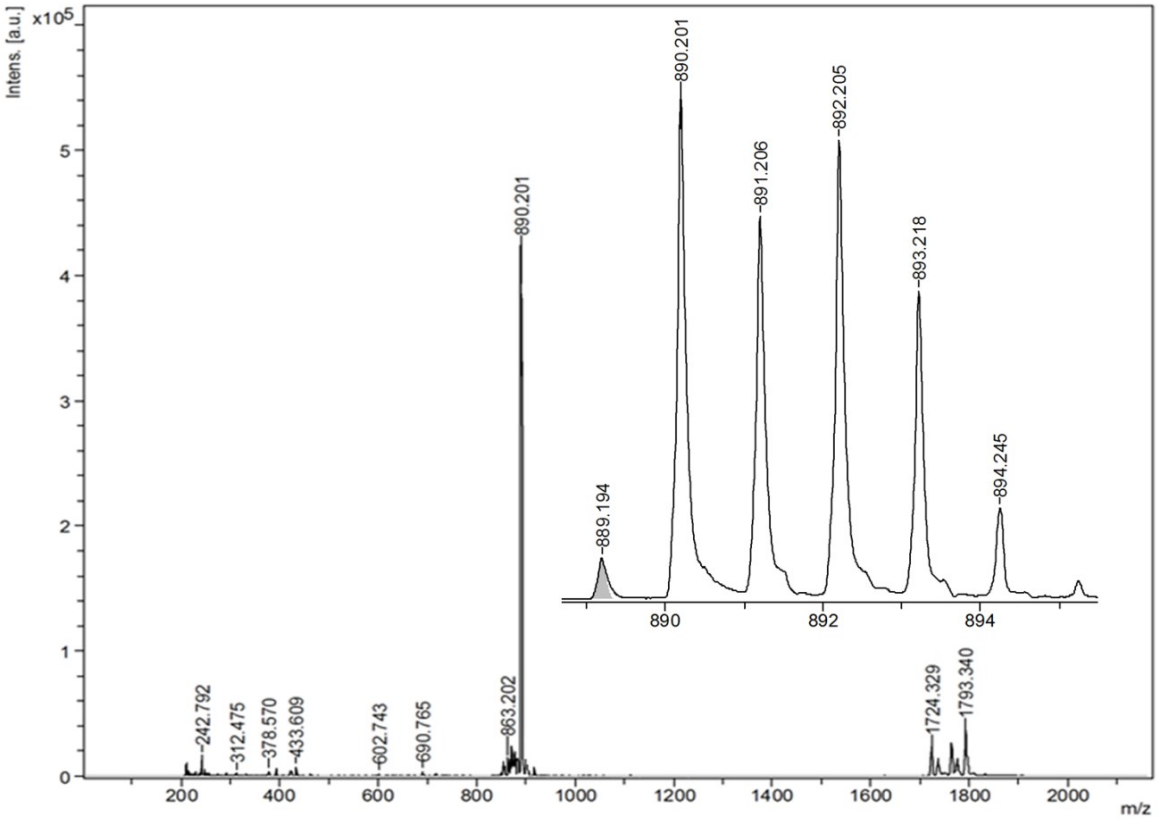

Fig. S2: Mass spectra of compound **3a.** Inset: represent isotopic pattern of molecular ion peak

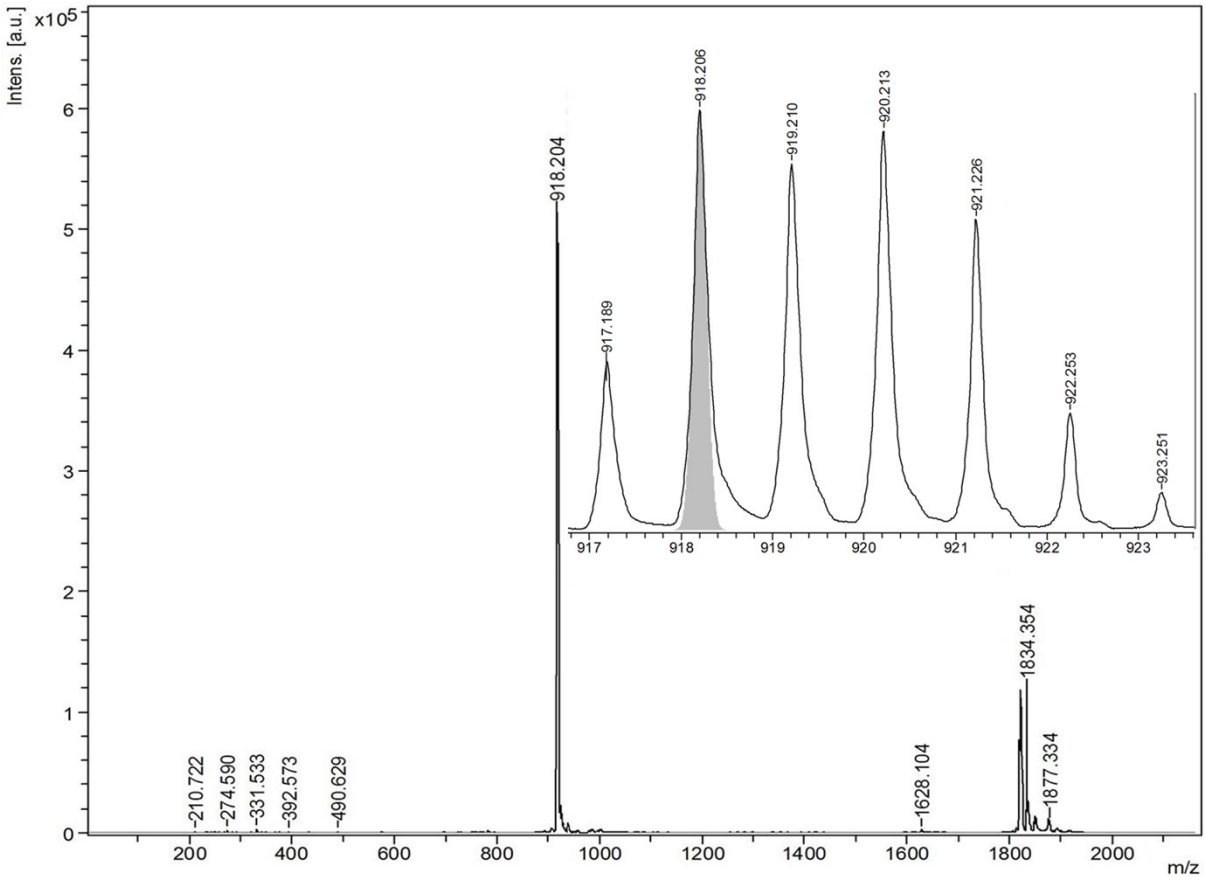

Fig. S3: Mass spectra of compound **3b.** Inset: represent isotopic pattern of molecular ion peak

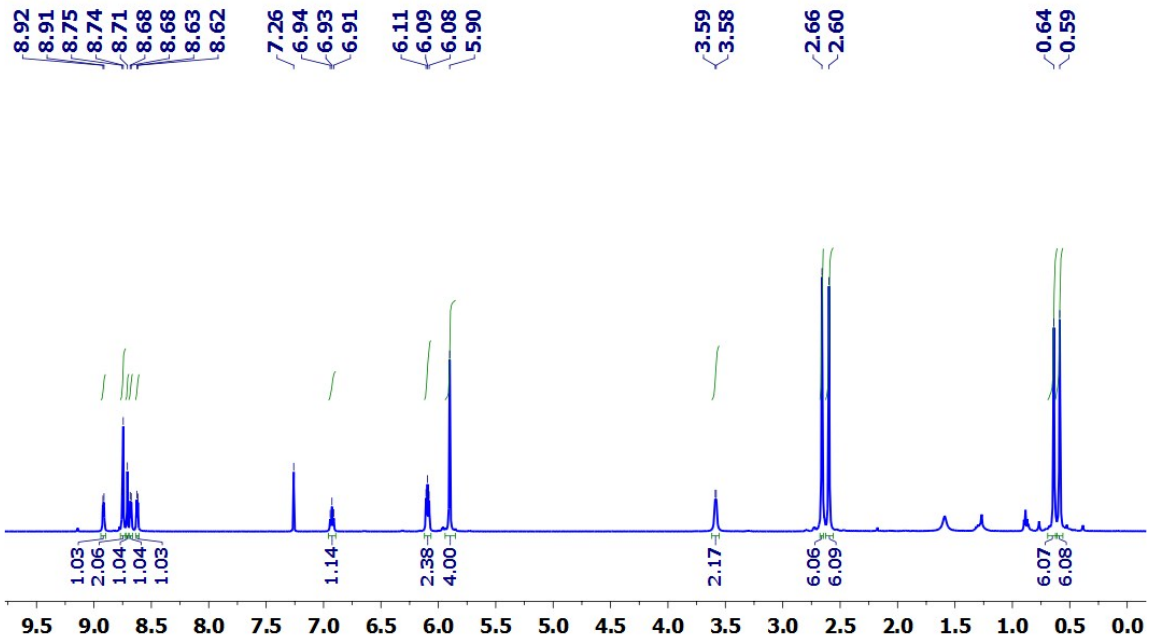

Fig. S4: ^{1}H-NMR of **4** in $CDCl_3$ at 298 K.

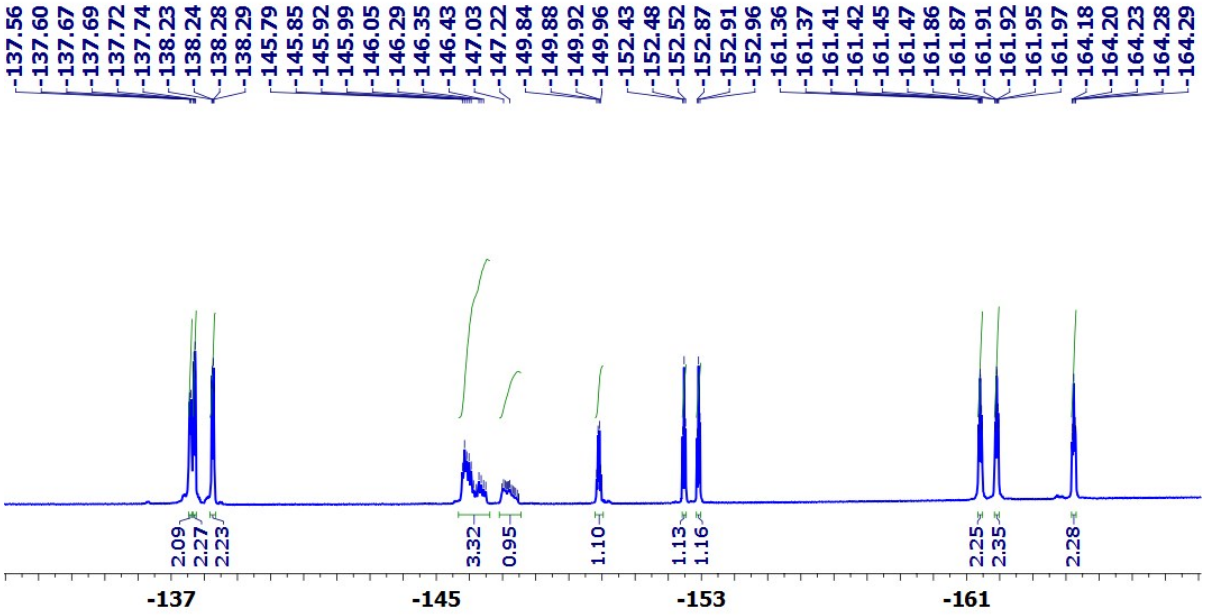

Figure S5: ^{19}F NMR of **4** in $CDCl_3$ at 298 K.

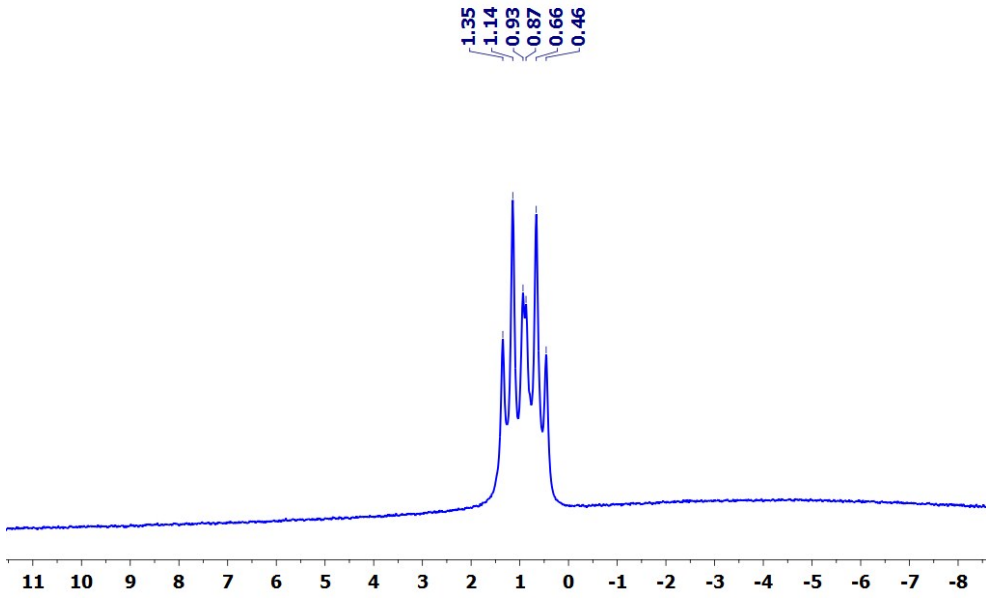

Fig. S6: ^{11}B-NMR of compound **4** in $CDCl_3$ at 298 K.

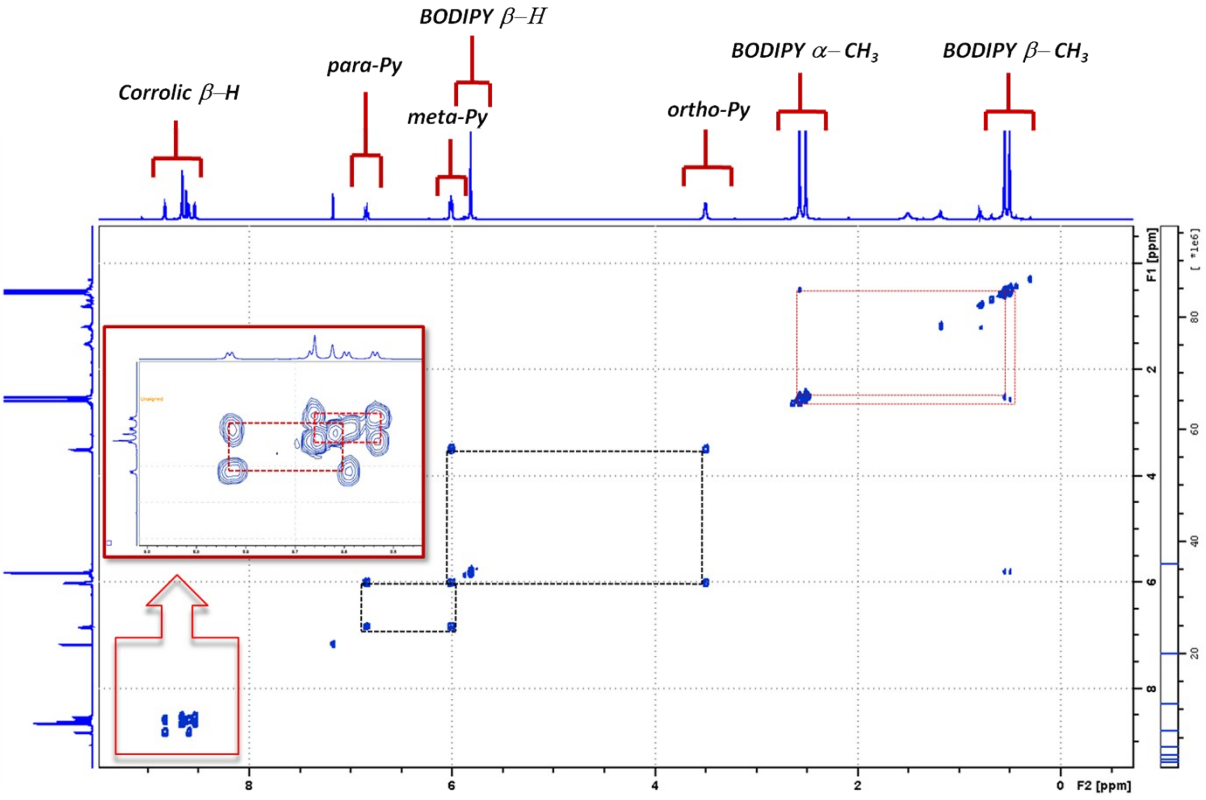

Fig. S7: ^{1}H-^{1}H COSY of compound **4** in $CDCl_3$ at 298 K.

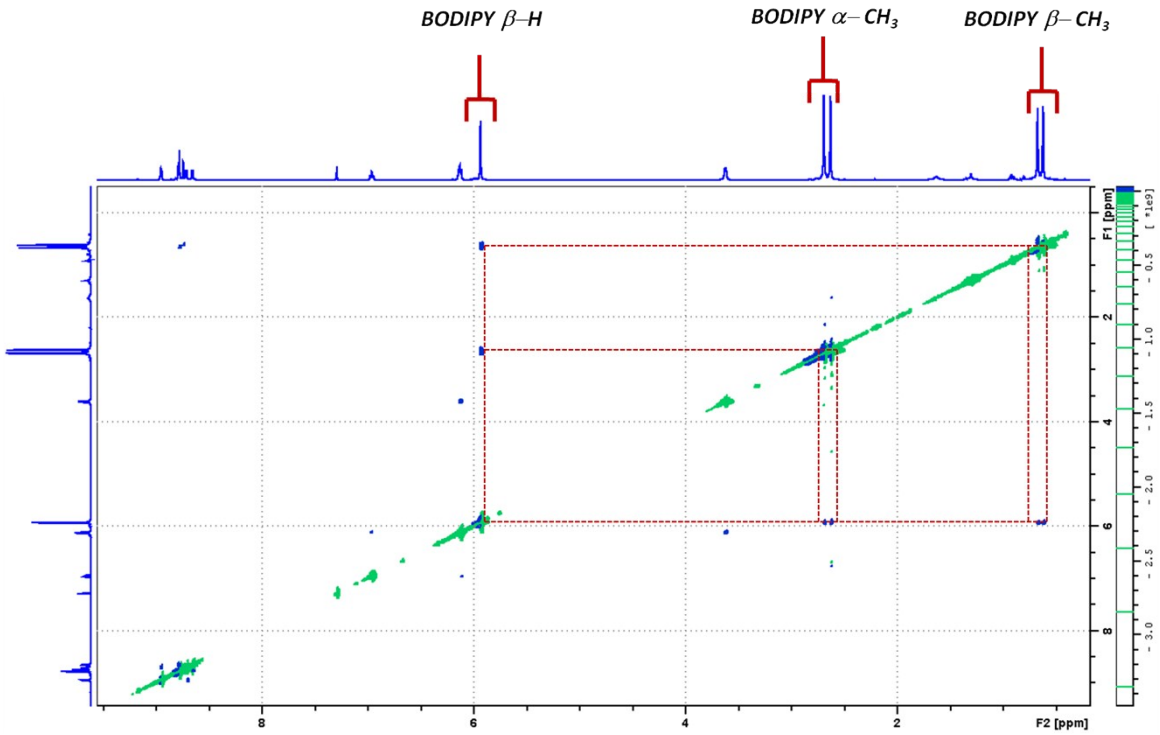

Fig. S8: ^{1}H-^{1}H ROESY of compound **4** in $CDCl_3$ at 298 K.

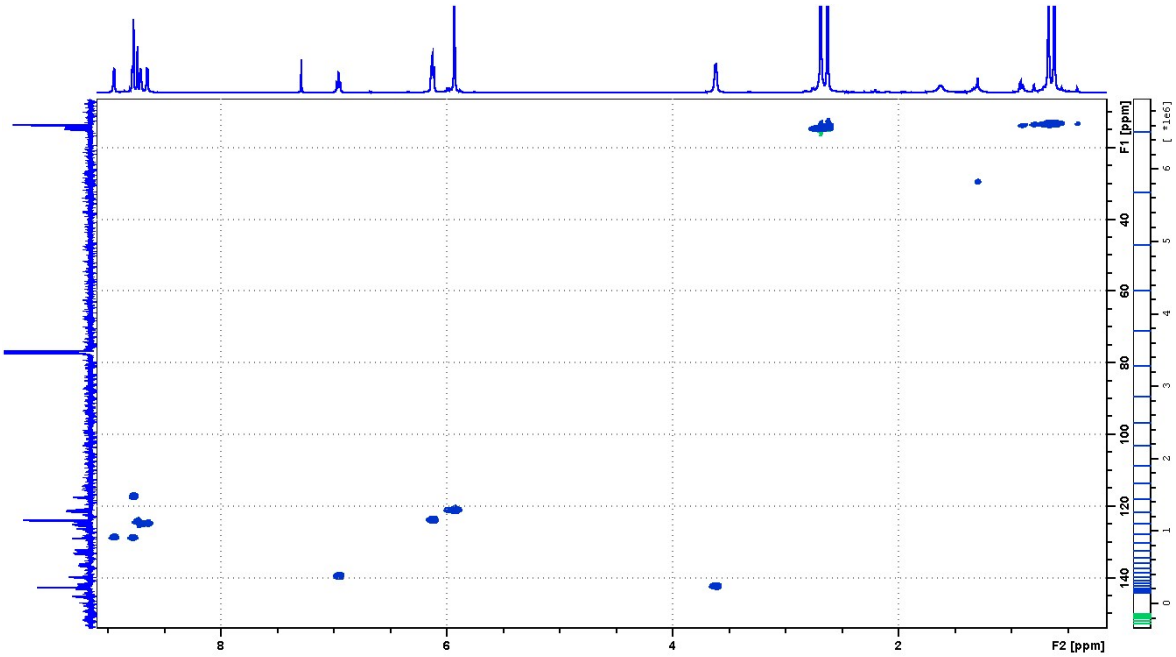

Fig. S9: ^{1}H-^{1}H HSQC of compound **4** in $CDCl_3$ at 298 K.

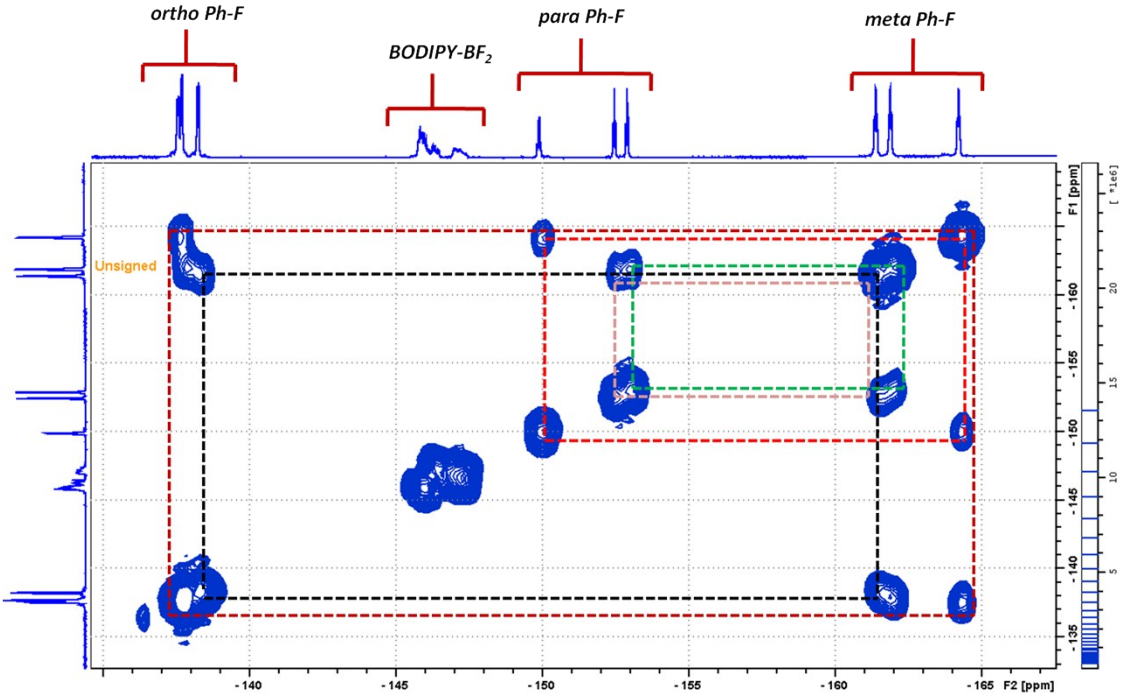

Fig. S10: ^{19}F-^{19}F COSY of compound **4** in $CDCl_3$ at 298 K.

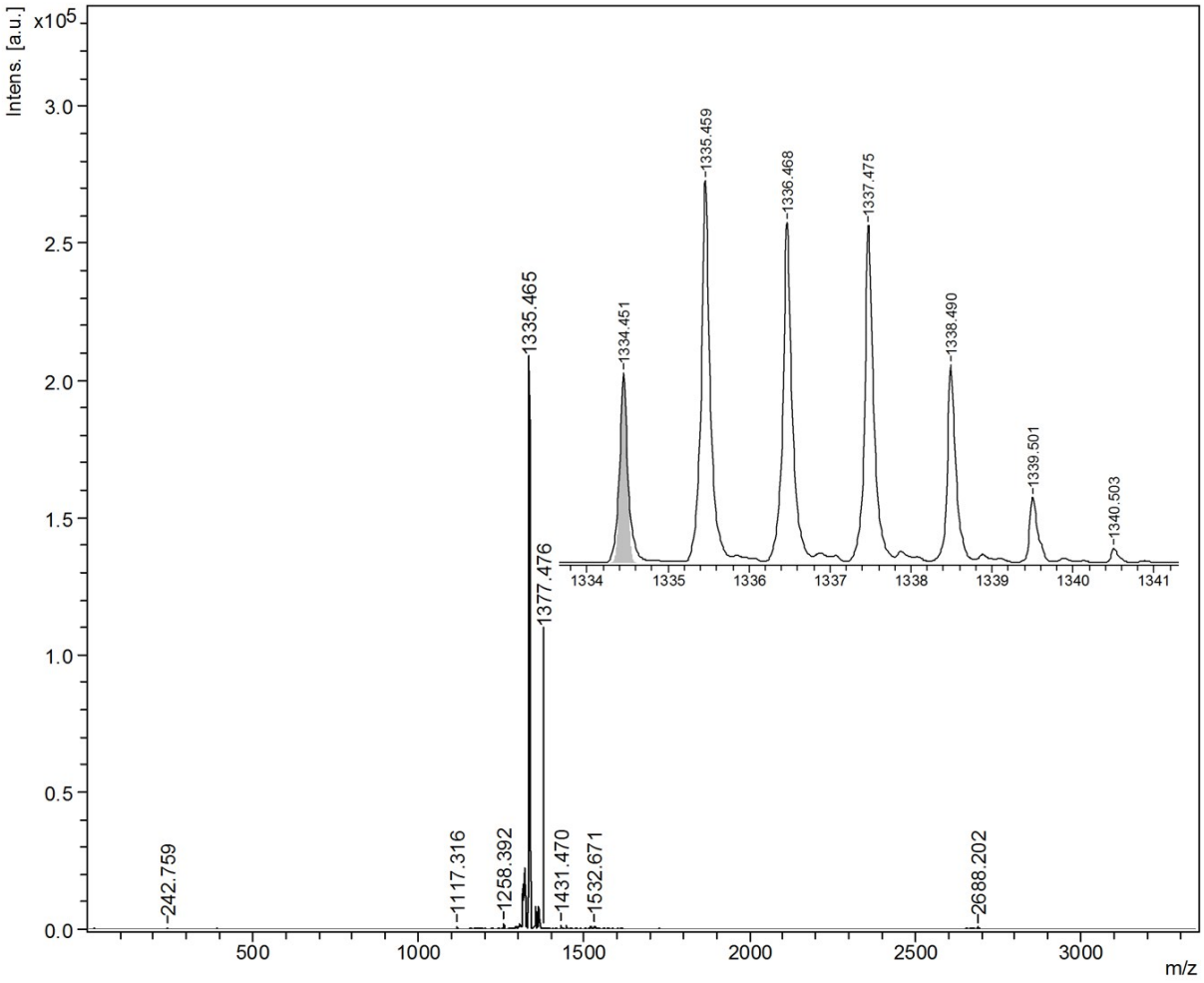

Fig. S11: MALDI-TOF (without matrix) mass spectra of compound **4**. Inset: represent isotopic pattern of molecular ion peak.

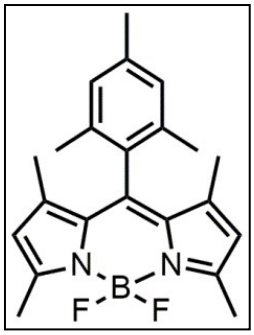

Fig. S12: Molecular structure of 4,4-difluoro-8-(2,4,6-trimethylphenyl)-1,3,5,7-tetramethyl-4-bora-3a,4a-diaza-*s*-indacene(**ref. BODIPY**).

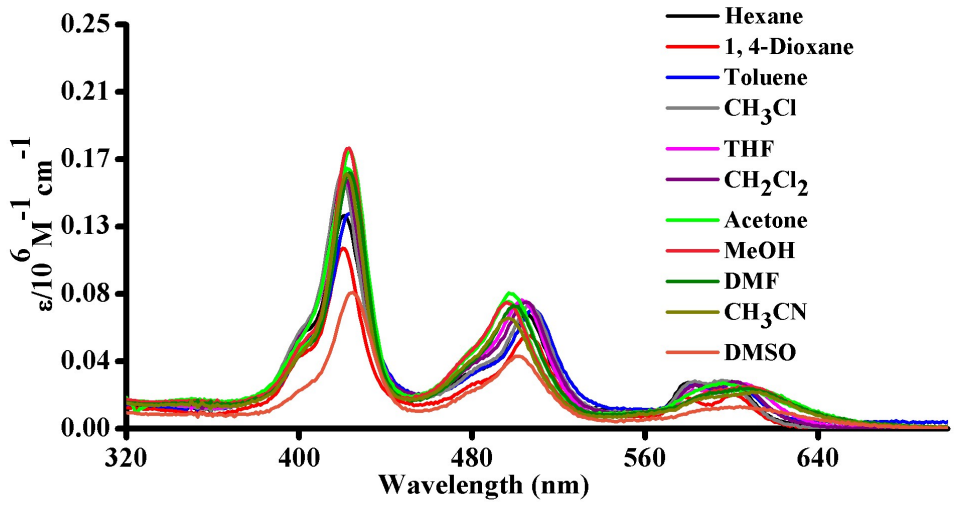

Fig. S13: UV-Vis absorption spectra of **4** (1.2x 10^{-6} M) in various solvents.

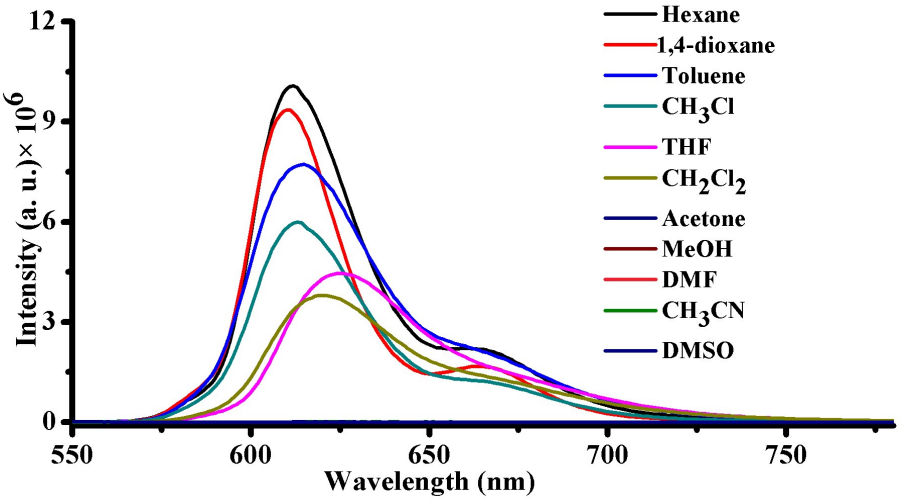

Fig. S14: Emission spectra of **4** (1.2x 10^{-6} M) in various solvents. Excitation λ = 423 nm

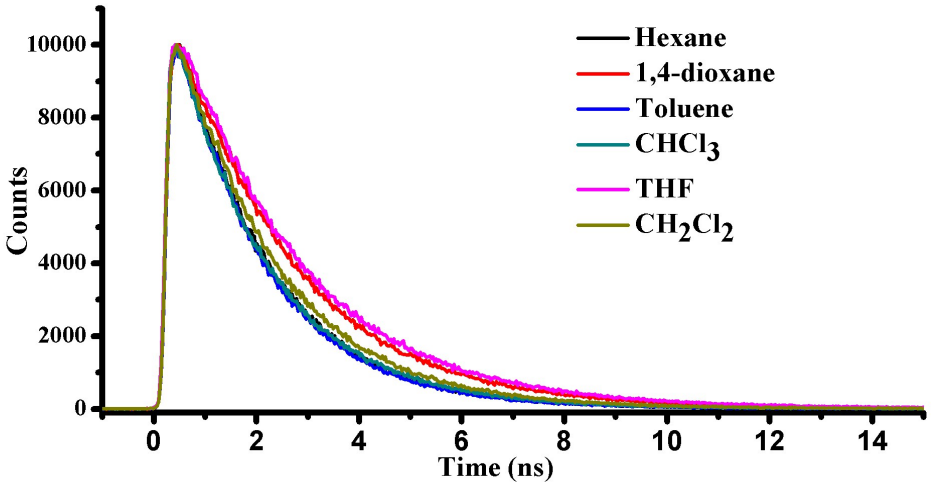

Fig. S15. Fluorescence emission decay plots of **4** in various solvents.

Table S1: Spectroscopy Data of Compound **4** in Various Solvent at 25°C.

Solvent	Dielectric constant(ε)[5]	λ_{max}, nm ($\varepsilon \times 10^{-4}$, M^{-1} cm^{-1})	λ_{em} (nm)[a]	Φ_{fl}[b]	τ (ns)
Hexane	1.89	421 (13.0), 505 (7.0), 580-600	611	0.118	1.78
1,4-Dioxane	2.21	421 (11.0), 506 (5.8), 578-602	610	0.129	2.28
Toluene	2.38	423 (13.2), 508 (7.3), 482-603	614	0.122	1.74
CH_3Cl	4.81	420 (15.6), 506 (7.6), 580-598	613	0.068	1.85
THF	7.52	422 (15.1), 503 (7.8), 582-608	625	0.063	2.40
CH_2Cl_2	9.14	420 (15.4), 504 (7.7), 581-604	620	0.054	1.94
Acetone	20.7	423 (16.8), 497 (7.8), 587-610	n.d[c]	-	-
MeOH	33.6	422 (17.3), 496 (7.7), 590-610	n.d	-	-
DMF	36.7	423 (15.7), 500 (7.6), 589-609	n.d	-	-
CH_3CN	37.5	422 (15.5), 497 (6.7), 586-612	n.d	-	-
DMSO	48.9	424 (8.3), 501 (4.5), 584-606	n.d	-	-

[a]Excitation at λ = 423 nm. [b]Quantum yield were measured with respect to Zn(TPP) in toluene, Φ_{fl} = 0.033. n.d = not detecteble. [c]very weak emission was detected.

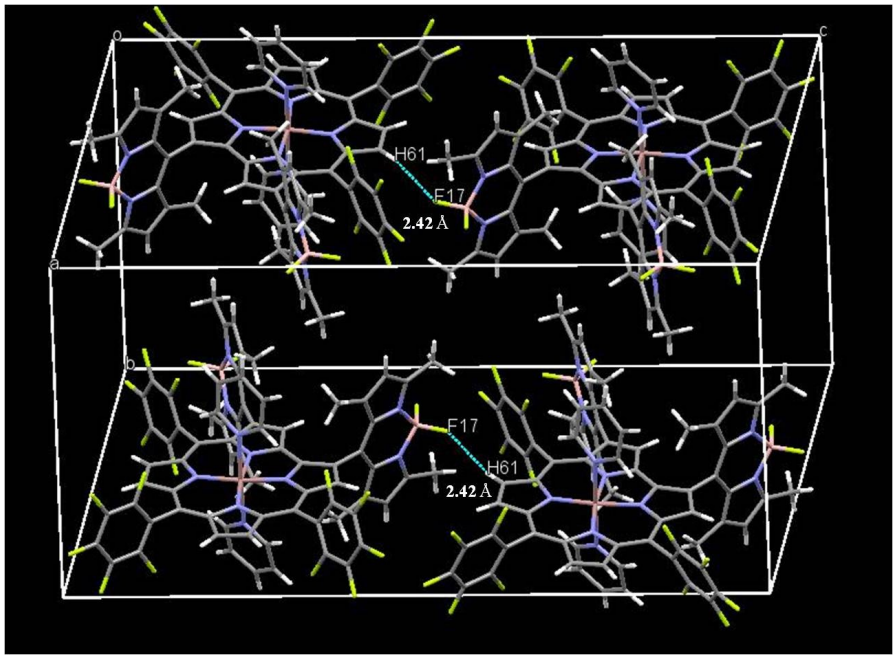

Fig. S16: Unit cell diagram of **4M.Py.Hex** showing intermolecular hydrogen bonding (C-H·····F). Solvent molecules were removed for clarity.

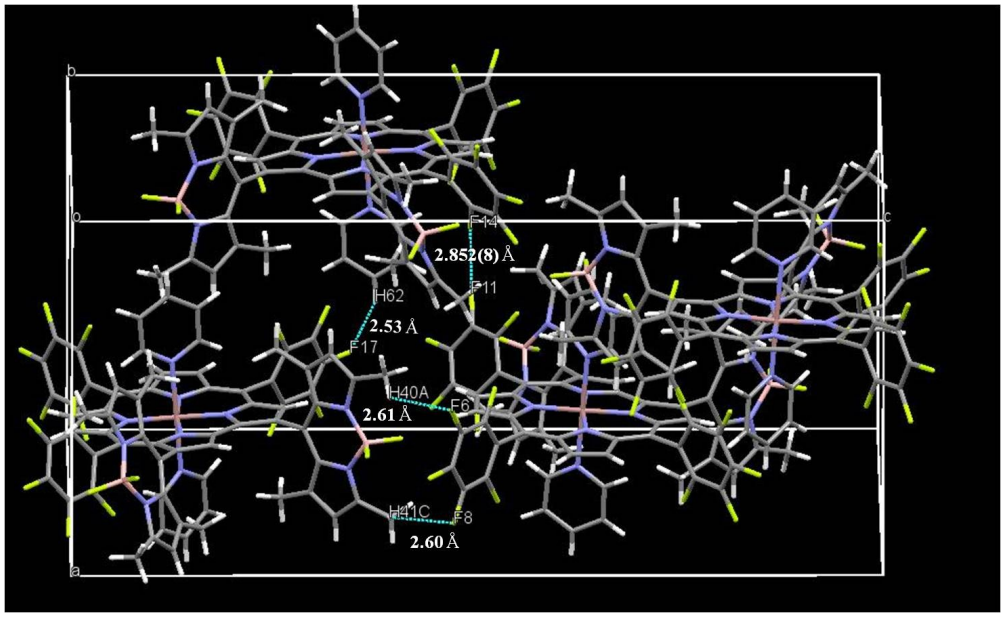

Fig. S17: Unit cell diagram of **4O.Py.Tol** showing intermolecular hydrogen bonding (C-H·····F) and C-F·····F-C contact. Solvent molecules were removed for clarity.

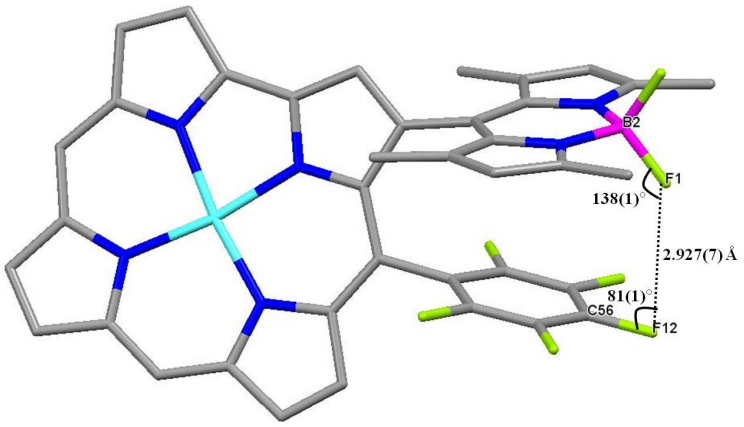

Fig. S18: Diagram representing intramolecular short C-H·····F-B contact in **4O.Py.Tol**. Solvent molecules, hydrogen and *meso*/*β*–substituents are omitted for clarity.

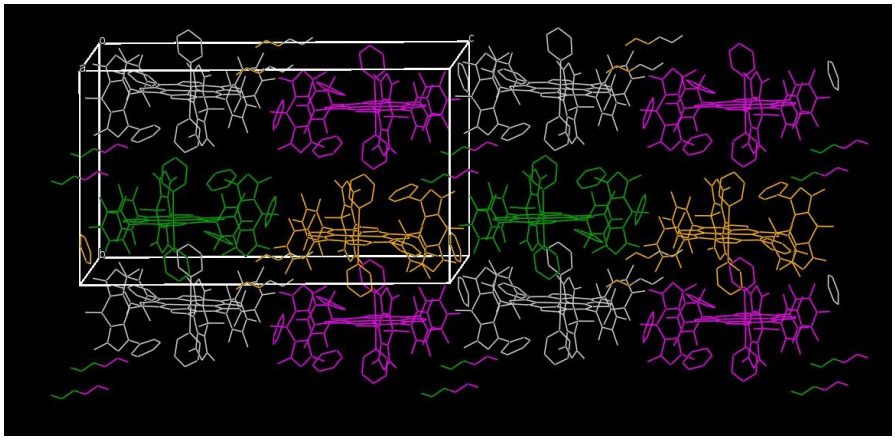

Fig. S19: Crystal packing diagram of **4M.Py.Hex.** Pyridine and hexane as lattice solvent molecules. Hydrogen molecules were removed for clarity.

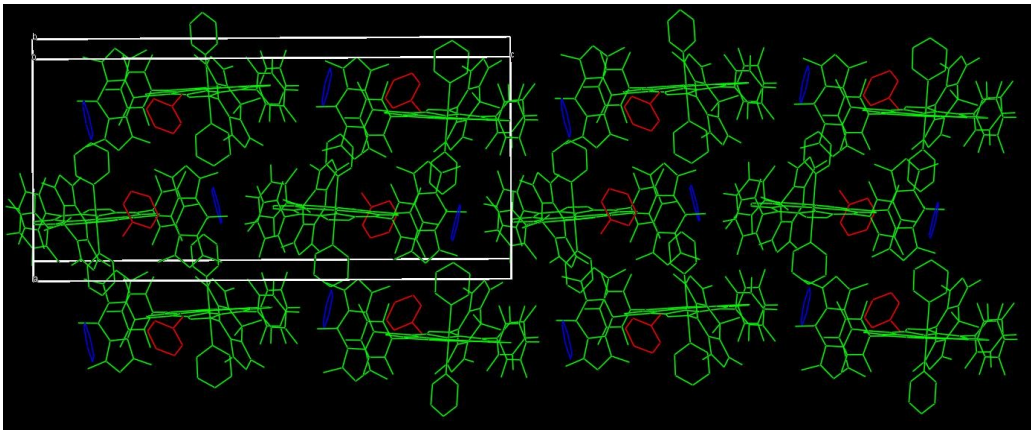

Fig. S20: Crystal packing diagram of **4O.Py.Tol.** Pyridine and toluene as lattice solvent molecules. Hydrogen molecules were removed for clarity.

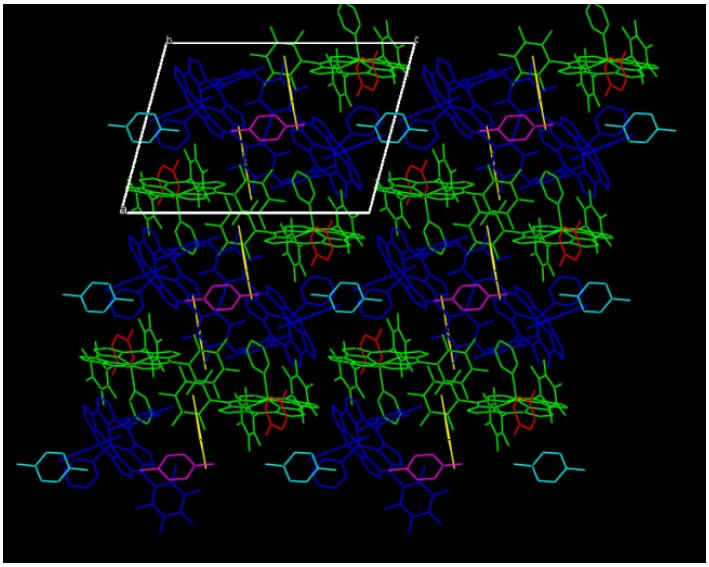

Fig. S21: Crystal packing diagram of **Ga(tpfc).Py (2)**. p-xylene as lattice solvent molecules.[6]

Table S2. Crystallographic data for compound **4** in monoclinic (**4M.Py.Hex**) and orthorhombic (**4O.Py.Tol**) crystal forms.

Data	**4M.Py.Hex**	**4O.Py.Tol**
Formula	'C91 H66 B2 F19 Ga N13'	'C85 H57 B2 F19 Ga N11'
Formula weight	1793.90	1684.75
Temperature/K	120(2)	100(2)
Wavelength (Å)	0.71073	0.71073
CCDC number	1425331	1411468
Crystal system	Monoclinic	Orthorhombic
Space group	$P2_1/c$	$P2_12_12_1$
a (Å)	16.260(6)	14.5257(16)
b (Å)	17.452(6)	16.4162(18)
c (Å)	29.954(9)	31.249(3)
α (˚)	90	90
β (˚)	97.616(11)	90
γ (˚)	90	90
V(Å^3)	8425(5)	7451.6(13)
Z	4	4
Density(g cm^{-3})	1.414	1.502
μ (mm^{-1})	0.424	0.473
F (000)	3660	3424
$h_{min, max}$, $k_{min, max}$, $l_{min, max}$	(-19, 19), (-21, 21), (-36, 36)	(-16, 16,), (-19, 19), (-36, 36)
No. of ref.	334319	164870
No. of unique ref./ obs. Ref.	16142, 11888	12354, 9066
No. parameters	1108	1002
R_{all}, R_{obs}	0.0957, 0.0658	0.1062, 0.0680
$wR2_{all}$, $wR2_{obs}$	0.1815, 0.1629	0.1761, 0.1570
$\Delta\rho_{min, max}$ (eÅ^{-3})	-0.537, 0.693	-0.400, 1.263
G. O. F.	1.050	1.043

Computational details:

All computational investigations were performed with Gaussian 09 program.[7] The calculations were performed by the density functional theory (DFT) method with restricted B3LYP (Becke's three parameter hybrid exchange functional and Lee−Yang−Parr correlation function) level, employing basis sets B3LYP/6-31G* (H, B, C, N, F) + LANL2DZ (Ga) level in vacuum, IEF-PCM (Toluene and DMSO).

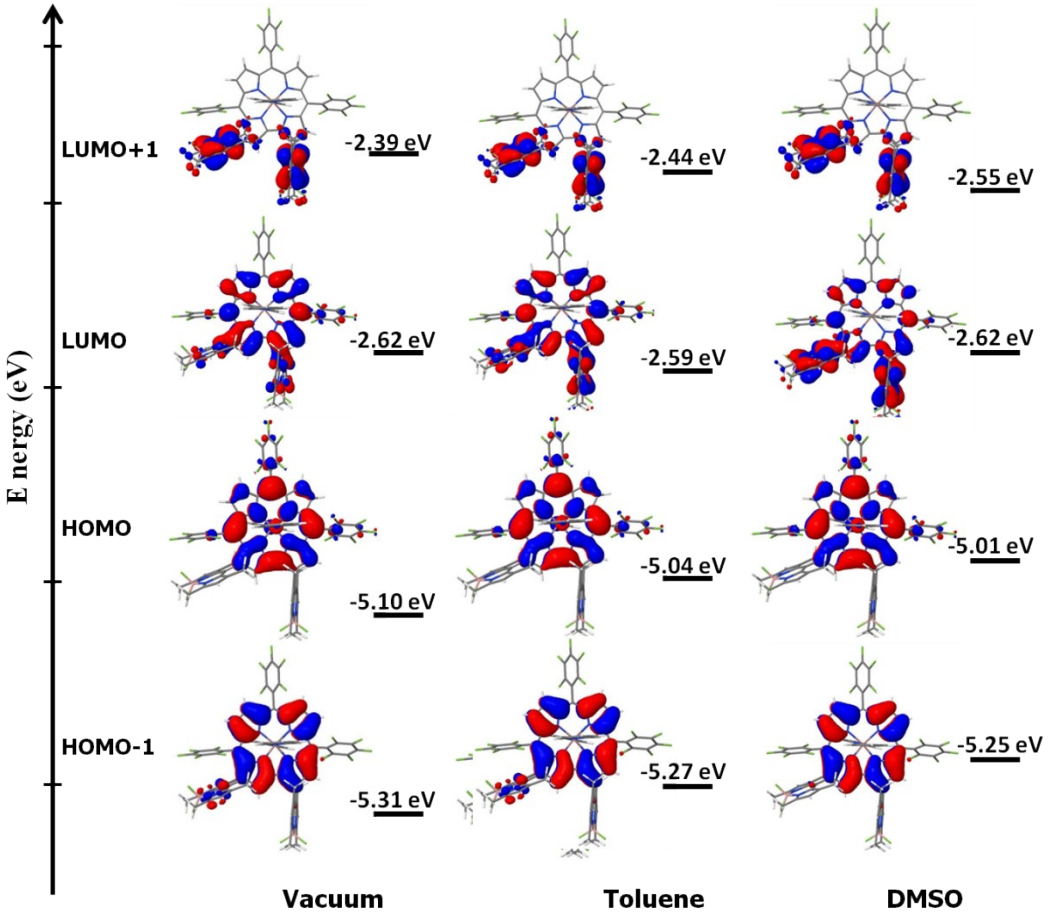

Fig. S22: Frontier molecular orbital plot of compound **4** in three dielectric medium obtained by DFT calculations at the B3LYP/6-31G* (H, B, C, N, F) + LANL2DZ (Ga) level in vacuum, IEF-PCM (Toluene and DMSO). Representations of energy levels are not to scale.

Table S3. ***List of Cartesian Coordinates for compound 4 in Vacuum:***

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.759831	1.224117	0.020035
2	6	0	-2.166392	1.434254	0.031320
3	6	0	-2.775676	0.179977	0.032837
4	6	0	-1.714009	-0.810566	0.020478
5	7	0	-0.538092	-0.122550	0.012483
6	6	0	-1.690756	-2.235988	0.005532
7	6	0	-0.506529	-3.014918	-0.007856

8	6	0	-0.416389	-4.453498	-0.045116
9	6	0	0.910560	-4.798014	-0.054533
10	6	0	1.681035	-3.581154	-0.021292
11	7	0	0.796094	-2.529401	0.005137
12	6	0	3.094121	-3.440677	-0.022272
13	6	0	3.809803	-2.216266	-0.019141
14	6	0	5.239211	-2.026095	0.014563
15	6	0	5.481440	-0.677992	0.016604
16	6	0	4.211552	0.004918	-0.016138
17	7	0	3.224668	-0.972286	-0.034785
18	6	0	3.986852	1.402486	-0.019586
19	6	0	2.695285	2.005048	-0.019820
20	6	0	2.254409	3.368991	-0.040081
21	6	0	0.858276	3.368331	-0.021950
22	6	0	0.452399	1.996864	0.006236
23	7	0	1.578716	1.228047	0.009370
24	6	0	-4.242847	-0.055179	0.038774
25	6	0	-4.957462	-0.017848	-1.173183
26	6	0	-4.904412	-0.296558	1.257850
27	6	0	-0.037284	4.550008	-0.023114
28	7	0	-6.275262	-0.580270	1.274790
29	6	0	-6.670399	-0.740505	2.553746
30	6	0	-5.561544	-0.547975	3.401811
31	6	0	-4.446376	-0.272638	2.617250
32	6	0	-4.552972	0.265459	-2.521486
33	6	0	-5.702037	0.159080	-3.296513
34	6	0	-6.778583	-0.192350	-2.457714
35	7	0	-6.332350	-0.287407	-1.189737
36	5	0	-7.166158	-0.795414	0.020170
37	9	0	-8.347997	-0.071680	0.135168
38	9	0	-7.444504	-2.160693	-0.138349
39	6	0	-3.073412	-0.002770	3.157367
40	6	0	-8.076966	-1.075787	2.930552
41	6	0	-3.200010	0.619398	-3.062289
42	6	0	-8.198629	-0.457285	-2.838840
43	6	0	-3.519522	-3.514344	1.177719
44	6	0	-4.733340	-4.194726	1.194184
45	6	0	-5.444339	-4.357460	0.007213
46	6	0	-4.931458	-3.849556	-1.183884
47	6	0	-3.711540	-3.180483	-1.172349
48	6	0	-2.983023	-2.982809	0.003027
49	9	0	-3.233997	-2.706730	-2.338070
50	9	0	-5.609720	-4.007803	-2.324380
51	9	0	-6.606681	-5.005325	0.011581
52	9	0	-5.222452	-4.686635	2.338498
53	9	0	-2.860846	-3.359493	2.341113
54	6	0	-0.248263	5.260691	1.171851
55	6	0	-0.669764	4.940201	-1.218491
56	7	0	-1.549672	6.028168	-1.231412
57	6	0	-2.014807	6.195263	-2.485033
58	6	0	-1.437904	5.218231	-3.321877
59	6	0	-0.589048	4.425795	-2.556058
60	6	0	0.234863	5.055514	2.508654
61	6	0	-0.317816	6.075544	3.274664
62	6	0	-1.123086	6.877904	2.439964

63	7	0	-1.081471	6.385695	1.186862
64	5	0	-1.889283	6.946506	-0.020818
65	9	0	-1.497540	8.256341	-0.291880
66	9	0	-3.254828	6.892545	0.253575
67	6	0	0.235279	3.293968	-3.095692
68	6	0	-2.983951	7.272867	-2.848762
69	6	0	1.124204	3.975556	3.052291
70	6	0	-1.927198	8.082475	2.807241
71	6	0	5.164540	2.311812	-0.005954
72	6	0	3.899513	-4.696890	-0.026327
73	6	0	6.024164	2.427031	-1.103909
74	6	0	7.116997	3.290403	-1.101888
75	6	0	7.368185	4.078000	0.019704
76	6	0	6.528513	3.993720	1.128601
77	6	0	5.447424	3.116967	1.103343
78	6	0	3.923449	-5.558539	1.077268
79	6	0	4.668496	-6.735412	1.084614
80	6	0	5.428152	-7.075362	-0.032212
81	6	0	5.431802	-6.239379	-1.146184
82	6	0	4.670637	-5.072842	-1.133121
83	9	0	4.668076	-7.534050	2.158639
84	9	0	6.150579	-8.198778	-0.034726
85	9	0	3.215018	-5.260969	2.176123
86	9	0	4.692412	-4.300457	-2.228720
87	9	0	6.156357	-6.566717	-2.222801
88	9	0	5.800236	1.697551	-2.208577
89	9	0	4.667511	3.048796	2.197606
90	9	0	6.772699	4.743329	2.208879
91	9	0	8.410648	4.911540	0.032117
92	9	0	7.917337	3.377495	-2.169882
93	1	0	-2.677600	2.387964	0.040730
94	1	0	-1.260653	-5.128651	-0.067663
95	1	0	1.318606	-5.798418	-0.090477
96	1	0	5.976964	-2.815699	0.043684
97	1	0	6.448863	-0.195651	0.046558
98	1	0	2.883371	4.249140	-0.069642
99	1	0	-5.586557	-0.602713	4.482721
100	1	0	-5.769837	0.313645	-4.365880
101	1	0	-3.110676	0.045676	4.250583
102	1	0	-2.658612	0.940050	2.787851
103	1	0	-2.368713	-0.794316	2.882097
104	1	0	-8.761676	-0.274789	2.633855
105	1	0	-8.154334	-1.233283	4.009512
106	1	0	-8.408824	-1.982516	2.412870
107	1	0	-2.442808	-0.115916	-2.775384
108	1	0	-3.240949	0.655897	-4.156000
109	1	0	-2.852644	1.595847	-2.707293
110	1	0	-8.482813	-1.480514	-2.567179
111	1	0	-8.334743	-0.325600	-3.915401
112	1	0	-8.878343	0.212076	-2.302753
113	1	0	-1.623687	5.118908	-4.383887
114	1	0	-0.169558	6.232757	4.335554
115	1	0	-0.107433	2.320126	-2.728860
116	1	0	0.172078	3.280447	-4.188690
117	1	0	1.289635	3.384346	-2.815321

118	1	0	-3.910124	7.168219	-2.273177
119	1	0	-2.572151	8.257820	-2.604865
120	1	0	-3.218273	7.233664	-3.915727
121	1	0	1.162570	4.049466	4.144262
122	1	0	2.150406	4.042380	2.675175
123	1	0	0.758470	2.975944	2.793637
124	1	0	-1.819245	8.305627	3.871834
125	1	0	-2.985708	7.920844	2.577338
126	1	0	-1.608334	8.952231	2.222723
127	31	0	1.320522	-0.686804	0.004537
128	6	0	2.207156	0.094709	3.035344
129	6	0	0.592888	-1.551544	3.055042
130	6	0	2.292214	0.091573	4.425692
131	1	0	2.824835	0.762960	2.445360
132	6	0	0.612203	-1.618519	4.446454
133	1	0	-0.066829	-2.190668	2.478388
134	1	0	2.984667	0.762525	4.923601
135	1	0	-0.040732	-2.316425	4.960250
136	6	0	0.349633	-1.342290	-3.040510
137	6	0	2.297541	-0.107880	-3.053018
138	6	0	0.324489	-1.403543	-4.432006
139	1	0	-0.425469	-1.820426	-2.451259
140	6	0	2.349945	-0.119534	-4.445142
141	1	0	3.067383	0.389987	-2.473370
142	1	0	-0.479796	-1.932358	-4.932990
143	1	0	3.167301	0.377424	-4.957529
144	6	0	1.344274	-0.780001	-5.149791
145	6	0	1.479254	-0.781739	5.147269
146	7	0	1.315797	-0.705617	-2.355713
147	7	0	1.373761	-0.711254	2.353804
148	1	0	1.521242	-0.809942	6.232442
149	1	0	1.356551	-0.810322	-6.235691

Table S4*: List of Cartesian Coordinates for compound 4 in Toluene:*

Center Numbe	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.761350	1.220477	0.014616
2	6	0	-2.166990	1.435172	0.028200
3	6	0	-2.779975	0.182155	0.029441
4	6	0	-1.721840	-0.811366	0.013286
5	7	0	-0.544334	-0.126996	0.004687
6	6	0	-1.702845	-2.237481	-0.005222
7	6	0	-0.521967	-3.020781	-0.020232
8	6	0	-0.436857	-4.460254	-0.059951
9	6	0	0.889003	-4.809035	-0.068172
10	6	0	1.663420	-3.593911	-0.031590
11	7	0	0.781856	-2.539613	-0.005558
12	6	0	3.077002	-3.457996	-0.028016
13	6	0	3.797656	-2.235692	-0.020074
14	6	0	5.228137	-2.051067	0.021444
15	6	0	5.475045	-0.703600	0.027269

16	6	0	4.207185	-0.016574	-0.010898
17	7	0	3.217190	-0.990261	-0.036757
18	6	0	3.987064	1.381564	-0.012384
19	6	0	2.697402	1.988631	-0.016494
20	6	0	2.263208	3.354503	-0.035958
21	6	0	0.866905	3.359383	-0.022299
22	6	0	0.454211	1.989523	0.003207
23	7	0	1.577317	1.216696	0.008142
24	6	0	-4.248056	-0.046108	0.043366
25	6	0	-4.969964	-0.006349	-1.164307
26	6	0	-4.905111	-0.278980	1.266578
27	6	0	-0.017087	4.549758	-0.025846
28	7	0	-6.279475	-0.549497	1.292566
29	6	0	-6.667282	-0.703878	2.575877
30	6	0	-5.551232	-0.520812	3.415516
31	6	0	-4.438294	-0.257148	2.622812
32	6	0	-4.569881	0.269340	-2.514992
33	6	0	-5.724741	0.173644	-3.284150
34	6	0	-6.800493	-0.163144	-2.439479
35	7	0	-6.348536	-0.261334	-1.172201
36	5	0	-7.178494	-0.751886	0.044482
37	9	0	-8.351369	-0.007667	0.165574
38	9	0	-7.488620	-2.112819	-0.108214
39	6	0	-3.059808	0.000876	3.154451
40	6	0	-8.073930	-1.021745	2.967732
41	6	0	-3.216133	0.607428	-3.063964
42	6	0	-8.225374	-0.408050	-2.816645
43	6	0	-3.540745	-3.509951	1.160748
44	6	0	-4.756238	-4.187200	1.172687
45	6	0	-5.462772	-4.348451	-0.016517
46	6	0	-4.943694	-3.843046	-1.205254
47	6	0	-3.722822	-3.176024	-1.189437
48	6	0	-2.998020	-2.979552	-0.011660
49	9	0	-3.242017	-2.704428	-2.354175
50	9	0	-5.618582	-4.001372	-2.349351
51	9	0	-6.628501	-4.993815	-0.017116
52	9	0	-5.251926	-4.677548	2.315805
53	9	0	-2.887657	-3.357456	2.326981
54	6	0	-0.230782	5.257309	1.170738
55	6	0	-0.628871	4.958729	-1.225615
56	7	0	-1.485447	6.066628	-1.243175
57	6	0	-1.929285	6.250764	-2.503982
58	6	0	-1.363747	5.265549	-3.337382
59	6	0	-0.543007	4.449700	-2.564360
60	6	0	0.233141	5.035265	2.510936
61	6	0	-0.312166	6.059257	3.278573
62	6	0	-1.093284	6.880939	2.441505
63	7	0	-1.045670	6.396992	1.183432
64	5	0	-1.817543	6.981438	-0.032114
65	9	0	-1.392481	8.287997	-0.288104
66	9	0	-3.192034	6.967282	0.220468
67	6	0	0.258819	3.299761	-3.098972
68	6	0	-2.866360	7.352326	-2.880461
69	6	0	1.100314	3.938590	3.056388
70	6	0	-1.878091	8.097055	2.813050

71	6	0	5.167530	2.287215	0.008672
72	6	0	3.878238	-4.716860	-0.030680
73	6	0	6.036066	2.397455	-1.082512
74	6	0	7.130997	3.257461	-1.073719
75	6	0	7.375790	4.046645	0.047500
76	6	0	6.527561	3.967185	1.149559
77	6	0	5.444199	3.094025	1.118173
78	6	0	3.894489	-5.581059	1.070726
79	6	0	4.635590	-6.759907	1.079381
80	6	0	5.399619	-7.100025	-0.033769
81	6	0	5.411303	-6.261886	-1.145451
82	6	0	4.653902	-5.093427	-1.133749
83	9	0	4.627201	-7.561148	2.152467
84	9	0	6.118812	-8.226384	-0.035010
85	9	0	3.181775	-5.283828	2.167769
86	9	0	4.683824	-4.319118	-2.228696
87	9	0	6.140561	-6.589384	-2.219851
88	9	0	5.819029	1.666317	-2.187706
89	9	0	4.655989	3.031117	2.206875
90	9	0	6.765762	4.719048	2.230607
91	9	0	8.421041	4.877775	0.066096
92	9	0	7.940294	3.339872	-2.136356
93	1	0	-2.676079	2.389912	0.040773
94	1	0	-1.282727	-5.133481	-0.085068
95	1	0	1.293346	-5.810984	-0.105828
96	1	0	5.963405	-2.842955	0.054122
97	1	0	6.444009	-0.224727	0.064058
98	1	0	2.896347	4.231746	-0.062295
99	1	0	-5.569465	-0.573835	4.496643
100	1	0	-5.796496	0.326627	-4.353469
101	1	0	-3.089279	0.046283	4.247841
102	1	0	-2.641261	0.941637	2.783944
103	1	0	-2.362557	-0.794503	2.871743
104	1	0	-8.751080	-0.207090	2.690761
105	1	0	-8.138595	-1.187486	4.046098
106	1	0	-8.427642	-1.919005	2.448281
107	1	0	-2.466363	-0.137761	-2.783388
108	1	0	-3.263654	0.647420	-4.157090
109	1	0	-2.854932	1.578081	-2.707262
110	1	0	-8.526152	-1.426148	-2.543724
111	1	0	-8.360710	-0.276978	-3.893167
112	1	0	-8.894884	0.274117	-2.283677
113	1	0	-1.538760	5.174768	-4.401935
114	1	0	-0.174006	6.206112	4.342260
115	1	0	-0.109152	2.334653	-2.733722
116	1	0	0.202603	3.287575	-4.192151
117	1	0	1.312756	3.365761	-2.810708
118	1	0	-3.795325	7.283810	-2.304308
119	1	0	-2.425681	8.329090	-2.653626
120	1	0	-3.102387	7.305345	-3.946491
121	1	0	1.129753	4.004988	4.148887
122	1	0	2.130282	3.993357	2.687774
123	1	0	0.722260	2.946582	2.787185
124	1	0	-1.776964	8.305217	3.881117
125	1	0	-2.937753	7.960597	2.572471

126	1	0	-1.535301	8.968513	2.244707
127	31	0	1.313369	-0.698142	-0.002264
128	6	0	2.195126	0.078164	3.030246
129	6	0	0.585501	-1.572302	3.045479
130	6	0	2.280219	0.071663	4.420505
131	1	0	2.811791	0.749575	2.443081
132	6	0	0.604680	-1.642926	4.436620
133	1	0	-0.072117	-2.212503	2.467820
134	1	0	2.971190	0.742468	4.920347
135	1	0	-0.045809	-2.344117	4.948735
136	6	0	0.348913	-1.342689	-3.046712
137	6	0	2.292499	-0.101471	-3.050554
138	6	0	0.323626	-1.394080	-4.438466
139	1	0	-0.424403	-1.827843	-2.461028
140	6	0	2.344627	-0.102614	-4.442666
141	1	0	3.061055	0.395039	-2.468279
142	1	0	-0.478208	-1.922314	-4.943679
143	1	0	3.159880	0.400784	-4.951773
144	6	0	1.341032	-0.761444	-5.152175
145	6	0	1.469412	-0.805566	5.140065
146	7	0	1.312961	-0.707679	-2.356502
147	7	0	1.363915	-0.728055	2.345280
148	1	0	1.511384	-0.836510	6.224896
149	1	0	1.353083	-0.783694	-6.238000

Table S5: ***List of Cartesian Coordinates for compound 4 in DMSO:***

Center Number	**Atomic Number**	**Atomic Type**	**Coordinates (Angstroms) X**	**Y**	**Z**
1	6	0	-0.770863	1.206704	0.010843
2	6	0	-2.178119	1.404902	0.022563
3	6	0	-2.776483	0.143887	0.027143
4	6	0	-1.707414	-0.836986	0.014709
5	7	0	-0.538745	-0.138491	0.005474
6	6	0	-1.670558	-2.264148	-0.000934
7	6	0	-0.481269	-3.033041	-0.016364
8	6	0	-0.378929	-4.472392	-0.054710
9	6	0	0.951007	-4.804855	-0.064858
10	6	0	1.710749	-3.579212	-0.030391
11	7	0	0.816379	-2.535588	-0.004372
12	6	0	3.122319	-3.426358	-0.027391
13	6	0	3.829548	-2.194801	-0.020219
14	6	0	5.258102	-1.993829	0.025536
15	6	0	5.488990	-0.642915	0.029303
16	6	0	4.212837	0.028851	-0.014802
17	7	0	3.234359	-0.956939	-0.041893
18	6	0	3.976087	1.424330	-0.019425
19	6	0	2.679249	2.016017	-0.024683
20	6	0	2.230056	3.376995	-0.044128
21	6	0	0.833675	3.364876	-0.029503
22	6	0	0.436414	1.990001	-0.003779
23	7	0	1.567820	1.231070	0.000841
24	6	0	-4.242472	-0.096274	0.039271

25	6	0	-4.963557	-0.063163	-1.169479
26	6	0	-4.901522	-0.328874	1.261705
27	6	0	-0.067068	4.541995	-0.030180
28	7	0	-6.276240	-0.604360	1.286322
29	6	0	-6.663918	-0.758960	2.571706
30	6	0	-5.549691	-0.570908	3.410996
31	6	0	-4.436571	-0.303182	2.618113
32	6	0	-4.561354	0.206094	-2.520394
33	6	0	-5.714801	0.102709	-3.292781
34	6	0	-6.791422	-0.231300	-2.449945
35	7	0	-6.342643	-0.321859	-1.178702
36	5	0	-7.173264	-0.796864	0.039277
37	9	0	-8.341221	-0.035773	0.158849
38	9	0	-7.513457	-2.154196	-0.109764
39	6	0	-3.060365	-0.037775	3.151975
40	6	0	-8.068874	-1.079994	2.967717
41	6	0	-3.207461	0.543448	-3.069062
42	6	0	-8.214877	-0.476465	-2.833349
43	6	0	-3.491299	-3.551089	1.175577
44	6	0	-4.704148	-4.232364	1.196636
45	6	0	-5.417243	-4.397860	0.012847
46	6	0	-4.907615	-3.893334	-1.179380
47	6	0	-3.688879	-3.222636	-1.173576
48	6	0	-2.958038	-3.019584	-0.000737
49	9	0	-3.221123	-2.750029	-2.342345
50	9	0	-5.593913	-4.051753	-2.318664
51	9	0	-6.585870	-5.042690	0.021582
52	9	0	-5.193524	-4.719725	2.344879
53	9	0	-2.834925	-3.392157	2.338548
54	6	0	-0.278106	5.255313	1.163999
55	6	0	-0.703315	4.931711	-1.223988
56	7	0	-1.587985	6.019326	-1.235558
57	6	0	-2.052716	6.184611	-2.494033
58	6	0	-1.471954	5.211206	-3.328560
59	6	0	-0.620650	4.419771	-2.561260
60	6	0	0.207971	5.052916	2.498820
61	6	0	-0.344771	6.074300	3.266842
62	6	0	-1.152573	6.874248	2.436456
63	7	0	-1.114781	6.381010	1.179013
64	5	0	-1.922864	6.927125	-0.025471
65	9	0	-1.550085	8.251033	-0.298179
66	9	0	-3.296324	6.878923	0.252796
67	6	0	0.204550	3.289941	-3.102348
68	6	0	-3.026055	7.255181	-2.868912
69	6	0	1.101221	3.976792	3.042545
70	6	0	-1.953546	8.077726	2.815735
71	6	0	5.146342	2.343449	0.000806
72	6	0	3.938707	-4.675613	-0.030108
73	6	0	6.016378	2.458398	-1.088238
74	6	0	7.101531	3.329711	-1.079742
75	6	0	7.335702	4.124335	0.038989
76	6	0	6.485977	4.040141	1.138618
77	6	0	5.411947	3.156387	1.108123
78	6	0	3.971587	-5.536368	1.072862
79	6	0	4.726175	-6.705839	1.080714

80	6	0	5.487421	-7.040081	-0.035360
81	6	0	5.483114	-6.205236	-1.148802
82	6	0	4.712662	-5.046242	-1.135653
83	9	0	4.732913	-7.504747	2.156589
84	9	0	6.219943	-8.158777	-0.037738
85	9	0	3.260691	-5.244403	2.173949
86	9	0	4.727140	-4.273954	-2.233954
87	9	0	6.210496	-6.527209	-2.227205
88	9	0	5.810395	1.720387	-2.191422
89	9	0	4.621559	3.089894	2.195032
90	9	0	6.714053	4.799129	2.218164
91	9	0	8.372986	4.967109	0.057106
92	9	0	7.913287	3.416835	-2.141439
93	1	0	-2.699088	2.353180	0.031121
94	1	0	-1.216178	-5.156507	-0.079506
95	1	0	1.367582	-5.801847	-0.103871
96	1	0	6.002587	-2.776929	0.065050
97	1	0	6.452066	-0.152721	0.071564
98	1	0	2.854313	4.260416	-0.072128
99	1	0	-5.568429	-0.622975	4.492102
100	1	0	-5.783932	0.248970	-4.363148
101	1	0	-3.092565	0.012992	4.244743
102	1	0	-2.644598	0.902068	2.776112
103	1	0	-2.360068	-0.832324	2.875031
104	1	0	-8.749814	-0.267065	2.694304
105	1	0	-8.129355	-1.243891	4.046261
106	1	0	-8.422602	-1.979906	2.452686
107	1	0	-2.458050	-0.200781	-2.785535
108	1	0	-3.253610	0.581206	-4.161945
109	1	0	-2.847508	1.514489	-2.712431
110	1	0	-8.524546	-1.488216	-2.547103
111	1	0	-8.340565	-0.363062	-3.912695
112	1	0	-8.886301	0.219666	-2.320566
113	1	0	-1.656819	5.110963	-4.390483
114	1	0	-0.193479	6.232176	4.327048
115	1	0	-0.144819	2.316439	-2.741274
116	1	0	0.146988	3.281800	-4.195151
117	1	0	1.256689	3.376069	-2.813639
118	1	0	-3.957031	7.151220	-2.300638
119	1	0	-2.621960	8.246756	-2.638593
120	1	0	-3.255384	7.203689	-3.935856
121	1	0	1.137275	4.048422	4.134204
122	1	0	2.126665	4.051582	2.665582
123	1	0	0.742030	2.976430	2.779105
124	1	0	-1.837130	8.291455	3.880793
125	1	0	-3.015520	7.921344	2.597683
126	1	0	-1.636737	8.954794	2.240770
127	31	0	1.326907	-0.687471	-0.005328
128	6	0	2.206582	0.106403	3.023177
129	6	0	0.605937	-1.553188	3.044683
130	6	0	2.288401	0.108670	4.413660
131	1	0	2.821285	0.778312	2.434728
132	6	0	0.622026	-1.615305	4.436134
133	1	0	-0.047070	-2.200863	2.470193
134	1	0	2.974025	0.786254	4.911245

135	1	0	-0.026029	-2.316219	4.951361
136	6	0	0.375246	-1.356072	-3.046830
137	6	0	2.273382	-0.045690	-3.050018
138	6	0	0.343409	-1.395412	-4.438785
139	1	0	-0.377941	-1.872738	-2.461870
140	6	0	2.317007	-0.031845	-4.442283
141	1	0	3.026674	0.474257	-2.468368
142	1	0	-0.442166	-1.946400	-4.944798
143	1	0	3.109258	0.506597	-4.951429
144	6	0	1.333073	-0.719584	-5.152519
145	6	0	1.480474	-0.768588	5.136857
146	7	0	1.320378	-0.693439	-2.355083
147	7	0	1.381322	-0.708649	2.339973
148	1	0	1.519554	-0.792283	6.221663
149	1	0	1.338450	-0.730112	-6.238256

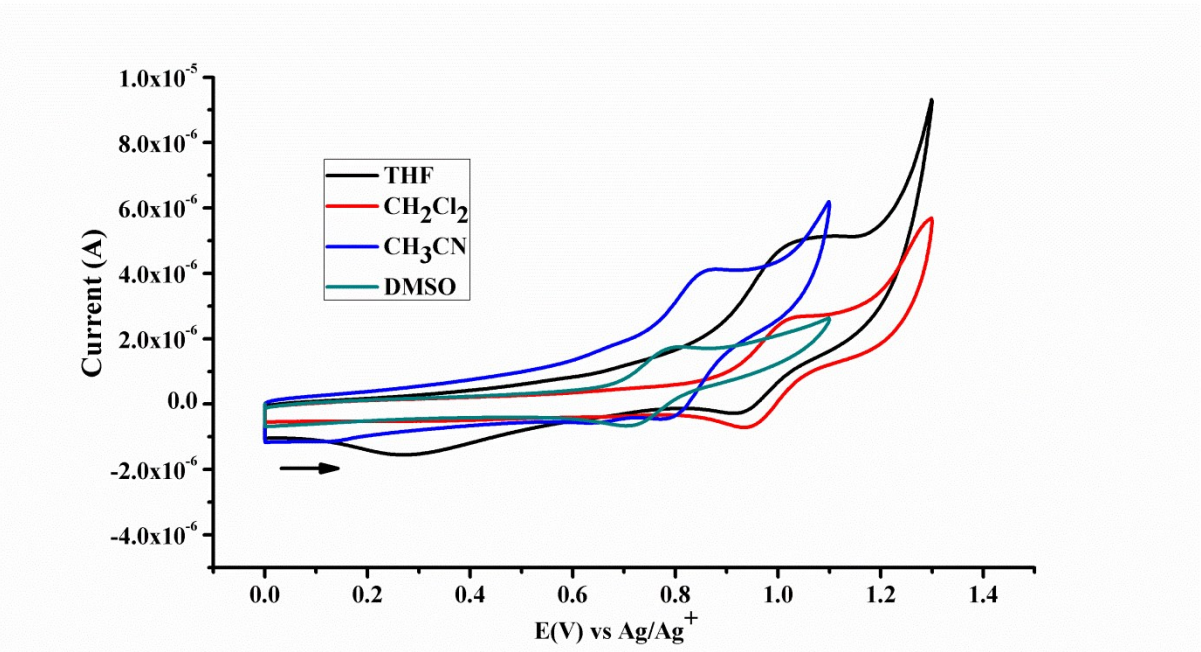

Fig. S23: Cyclic voltammograms of **4** in various solvents. Scan rate at 0.1V/s. Contain TBAPF (0.1 M) as supporting electrolyte.

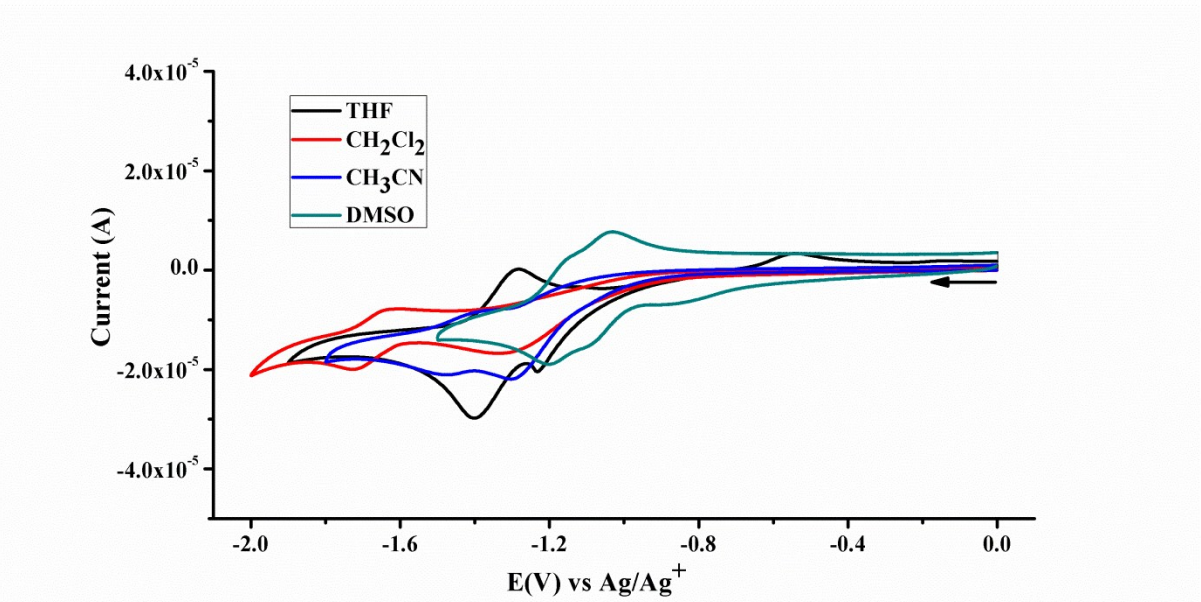

Fig. S24: Cyclic voltammograms of compound **4** in various solvents. Scan rate at 0.1V/s. Contain TBAPF (0.1 M) as supporting electrolyte.

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