Electronic Supplementary Material (ESI) for Polymer Chemistry.

Flexibility-driven 1D-structural preference in *bis*-terpyridine-Fe(II)-Metallo-supramolecular polymer possessing potential tricolor electrochromism

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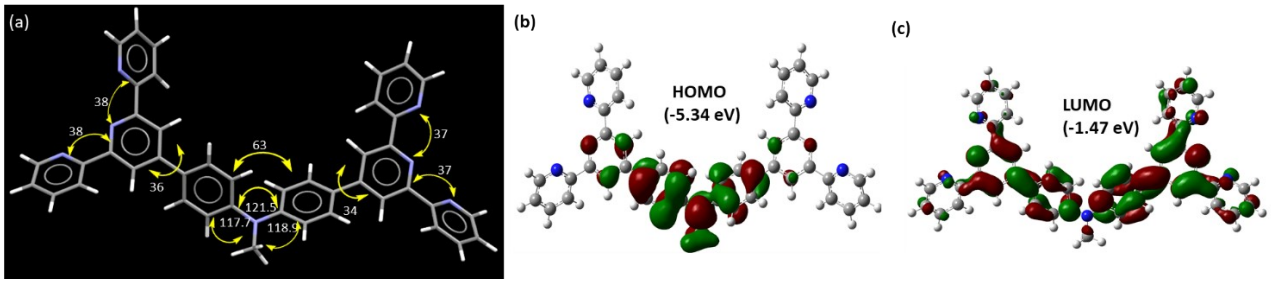

Fig S1: (a) DFT optimized structure using B3lyp/6-31g(d) functional; the angles (°) are determined using mercury software. For the simplicity of DFT calculation, the N-alkyl chain is truncated to N-Methyl. (b) HOMO (Highest occupied molecular orbital) (c) LUMO (Lowest unoccupied molecular orbital) with their individual energy in eV for DPATPY.

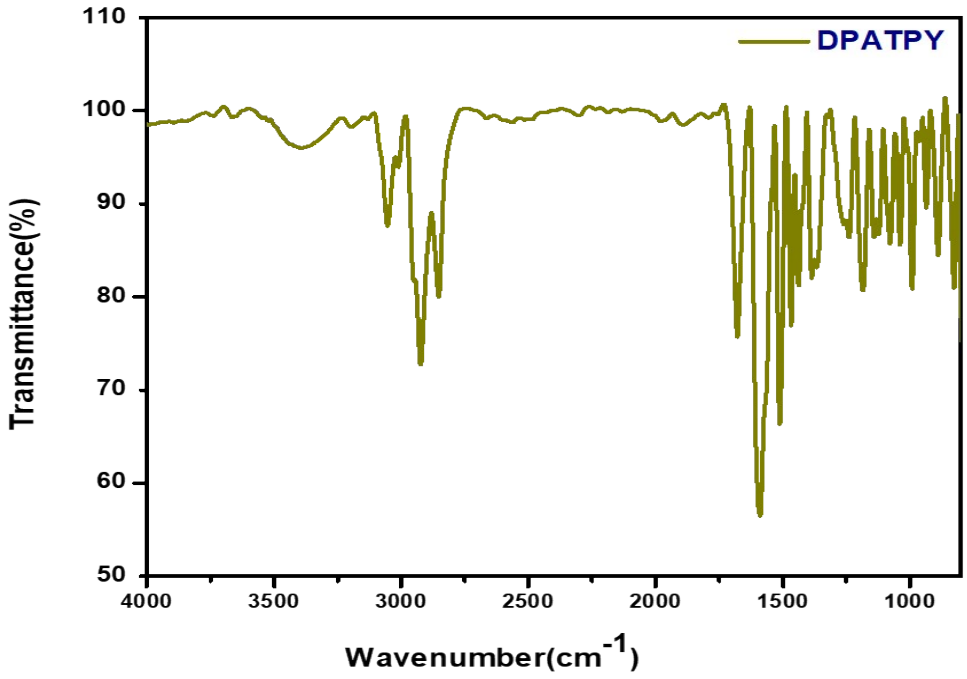

Fig. S2: FT-IR spectrum of **DPATPY**

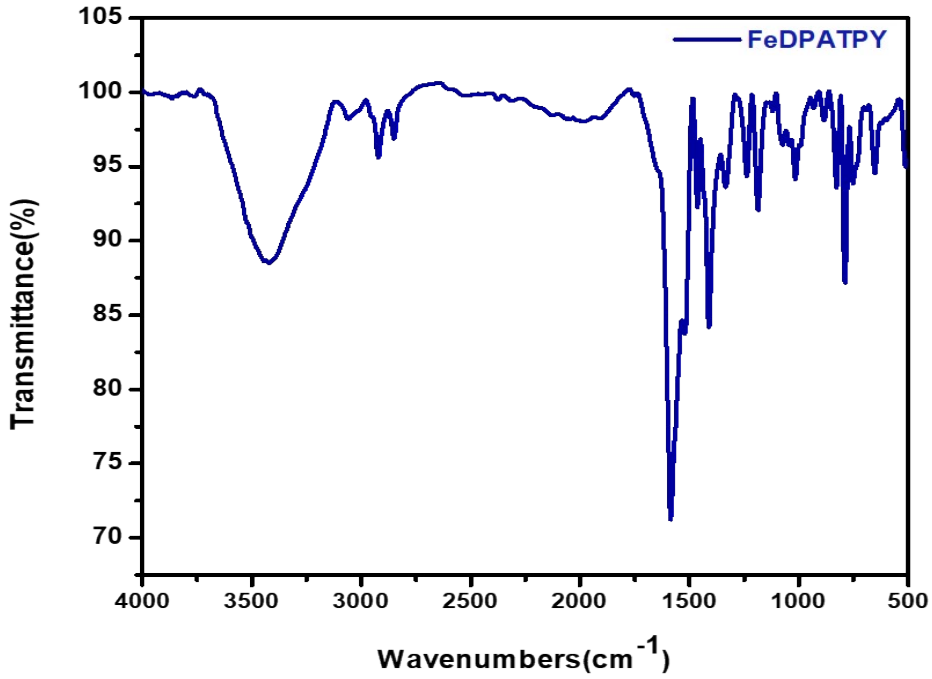

Fig. S3: FT-IR spectrum of **Fe-DPATPY**

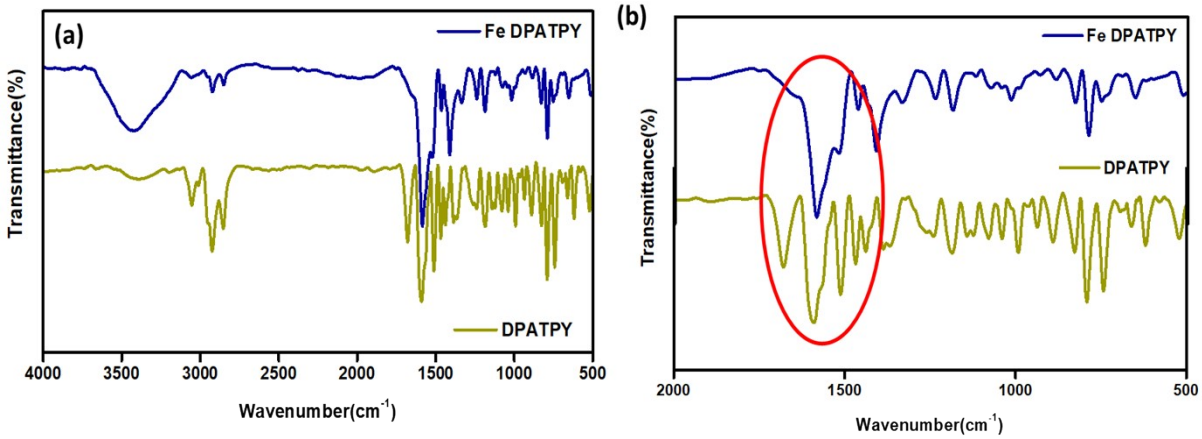

Fig. S4: Comparative FT-IR spectra of **DPATPY** and **Fe-DPATPY** (a) Full IR spectra (b) expanded spectra from 2000 to 500 cm^{-1}.

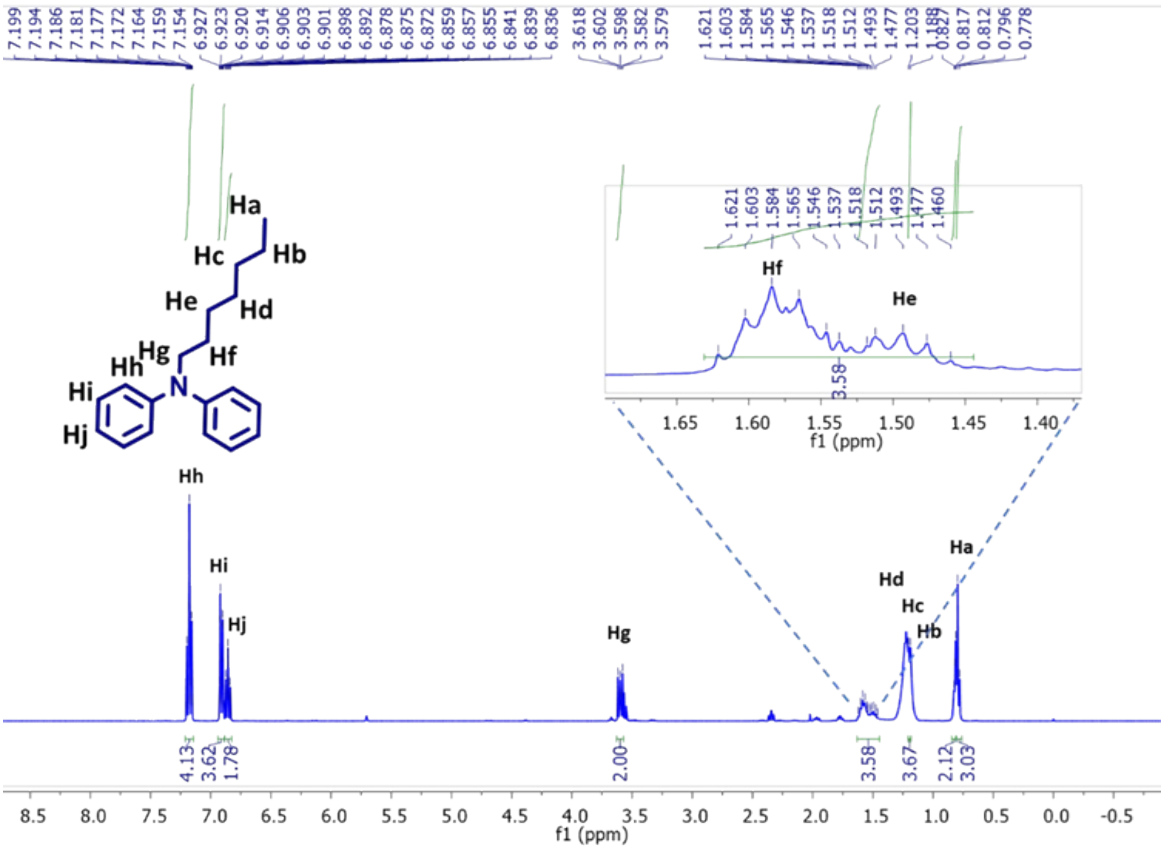

Fig.S5: ^{1}H NMR spectrum of **N-heptyl diphenylamine** (1) in $CDCl_3$

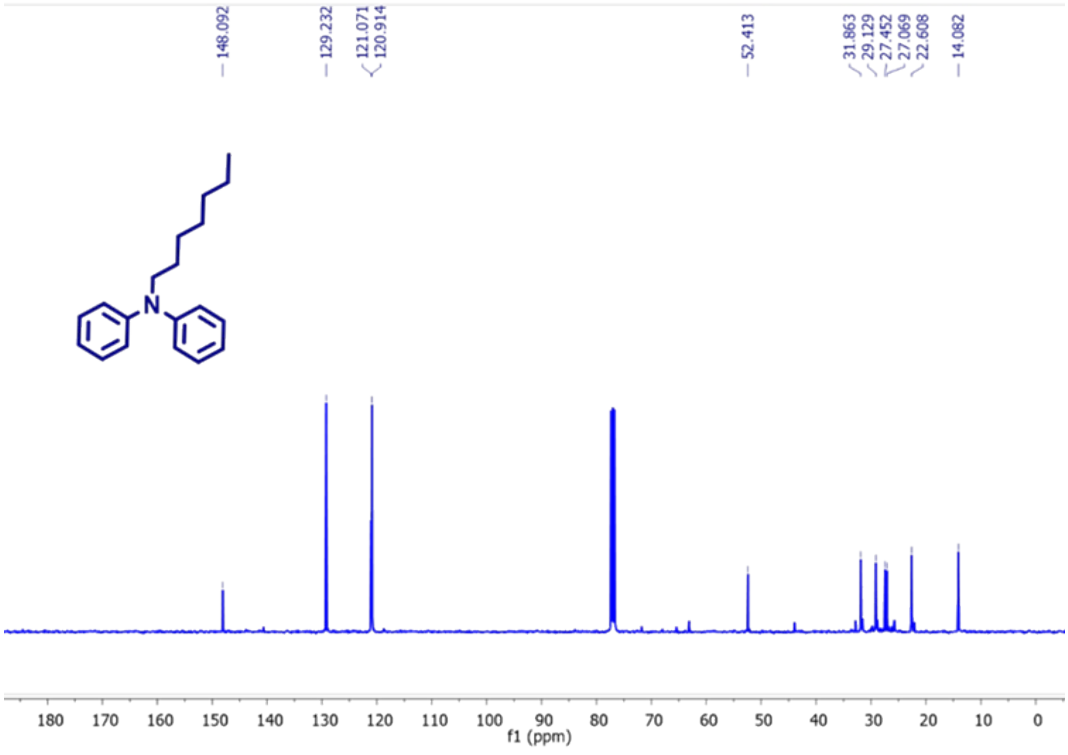

Fig.S6: ^{13}C NMR spectrum of **N-heptyl diphenylamine** (1) in $CDCl_3$

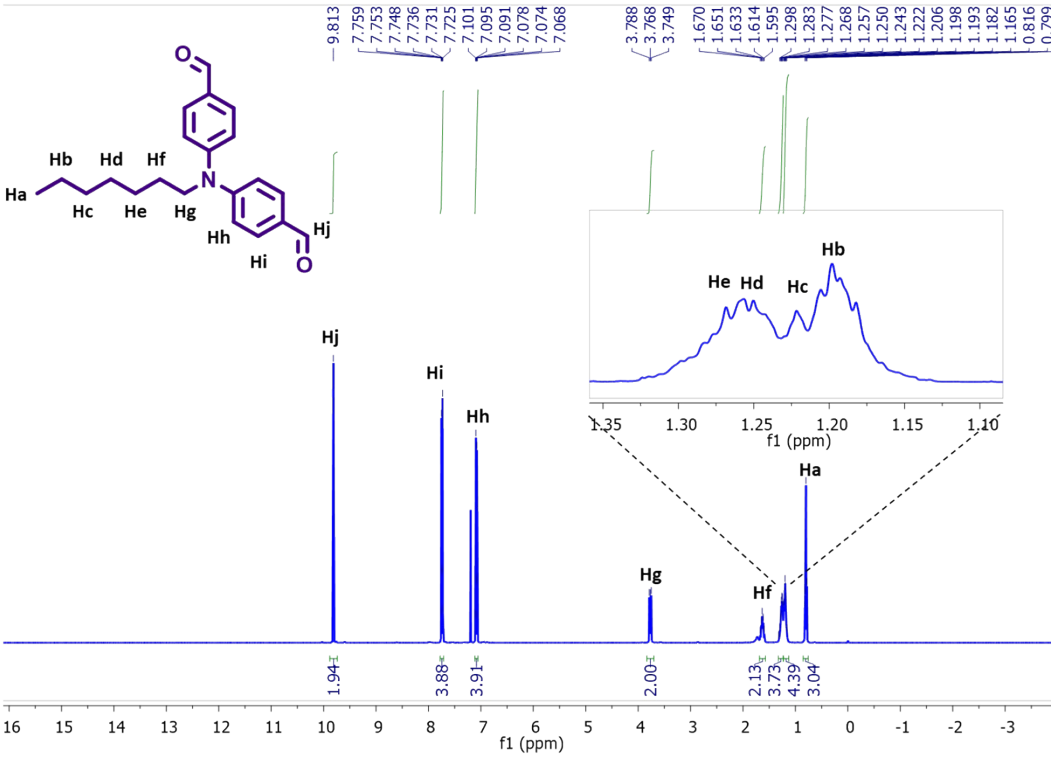

Fig.S7: ^{1}H NMR of N-heptyl DPA dialdehyde; **DPACHO** in $CDCl_3$

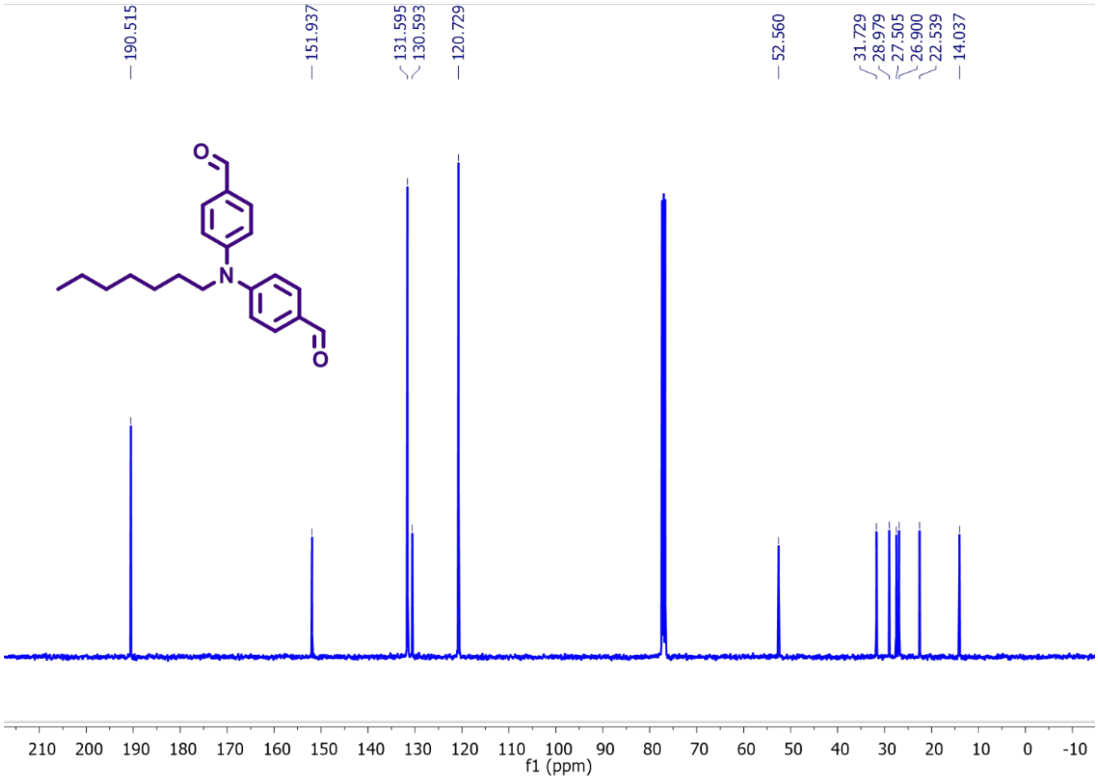

Fig.S8: ^{13}C-NMR of N-heptyl DPA dialdehyde; **DPACHO** in $CDCl_3$

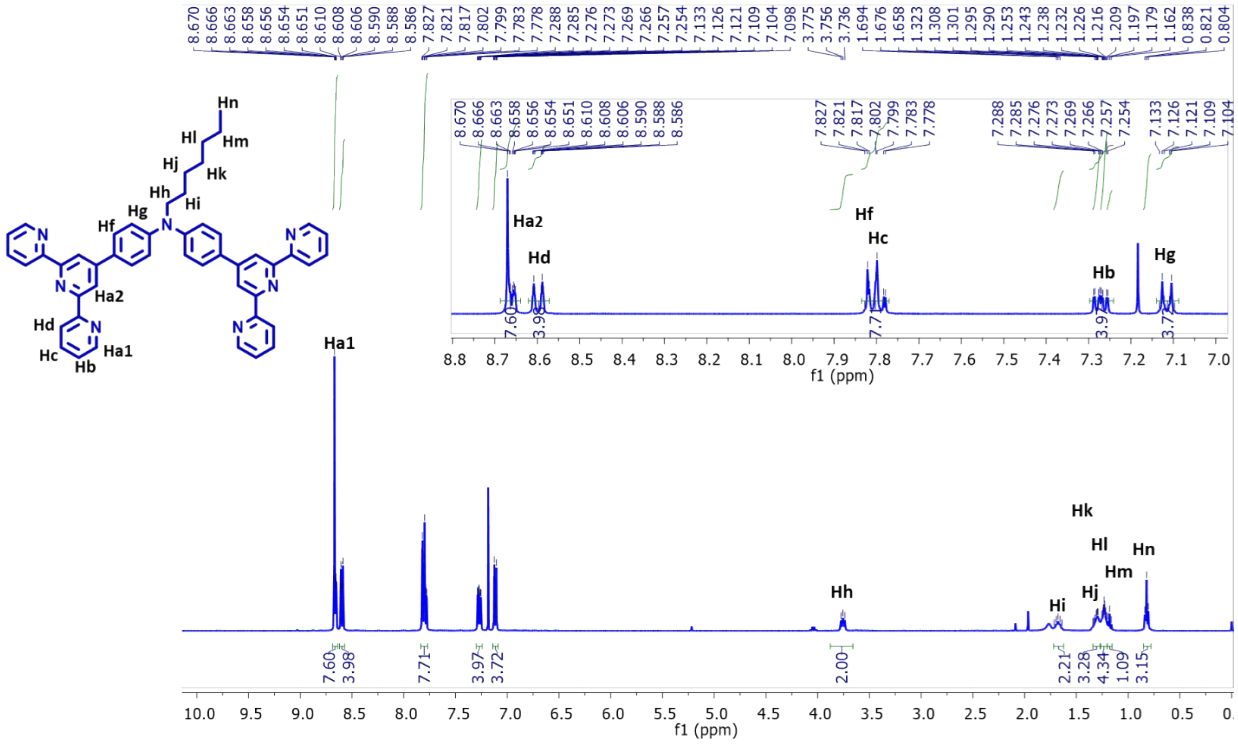

Fig. S9: ^{1}H-NMR spectrum of **DPATPY** in $CDCl_3$.

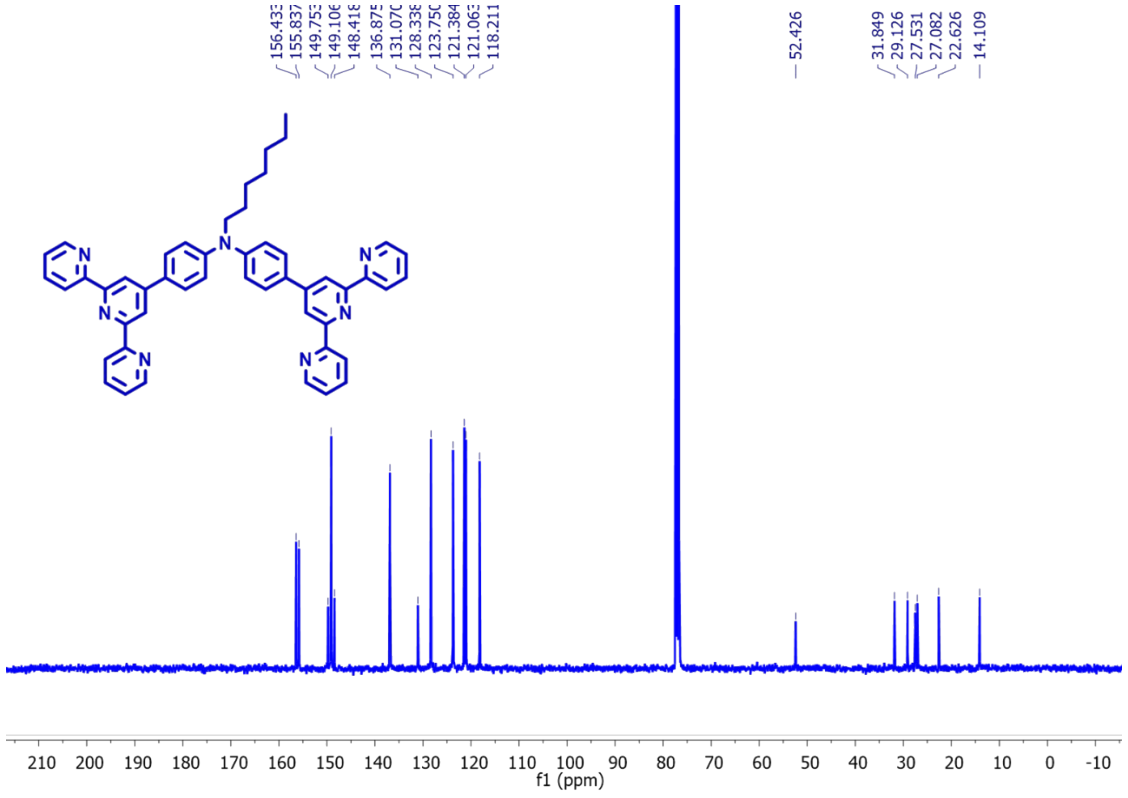

Fig. S10: ^{13}C-NMR spectrum of **DPATPY** in $CDCl_3$.

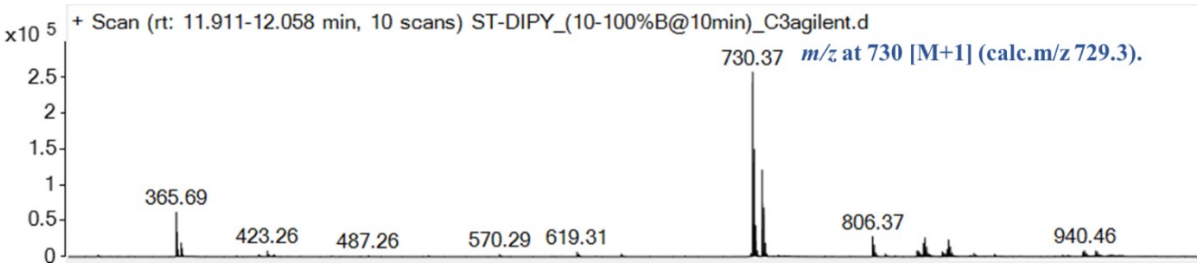

Fig. S11: ESI- MS spectrum of **DPATPY**

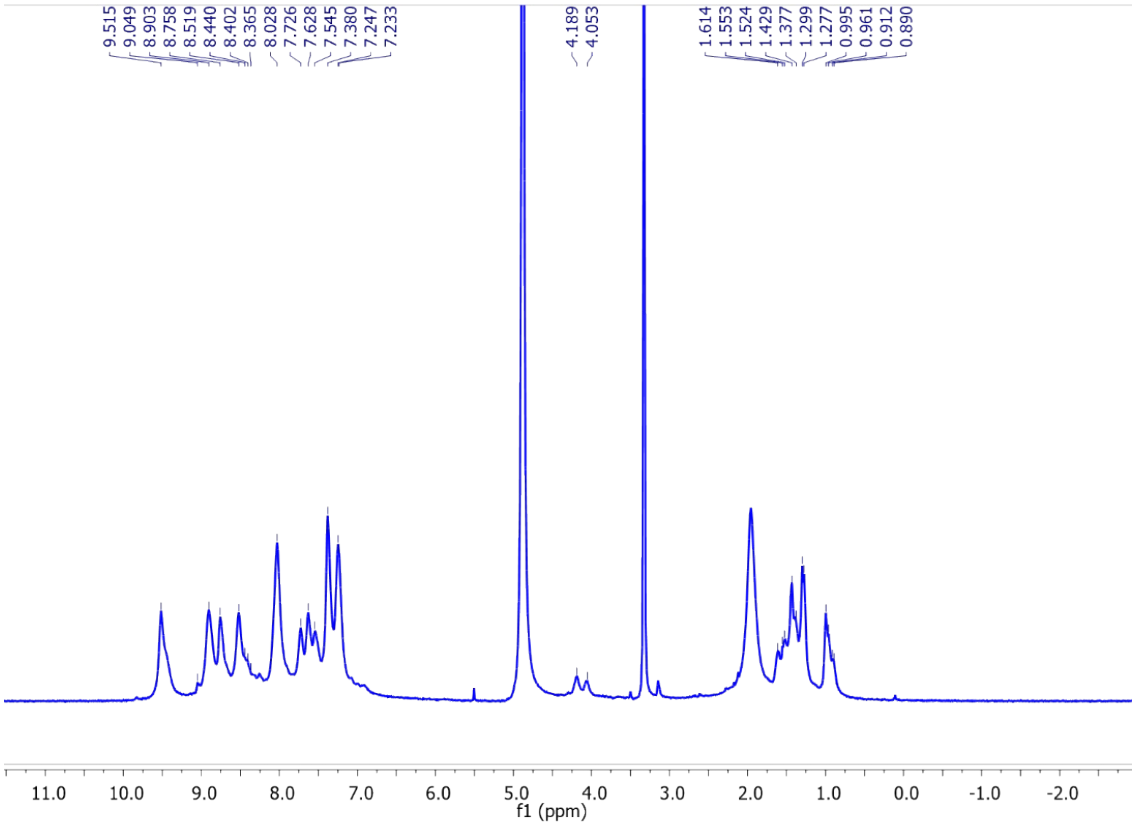

Fig. S12: ^{1}H NMR spectrum of **FeDPATPY** in CD_3OD

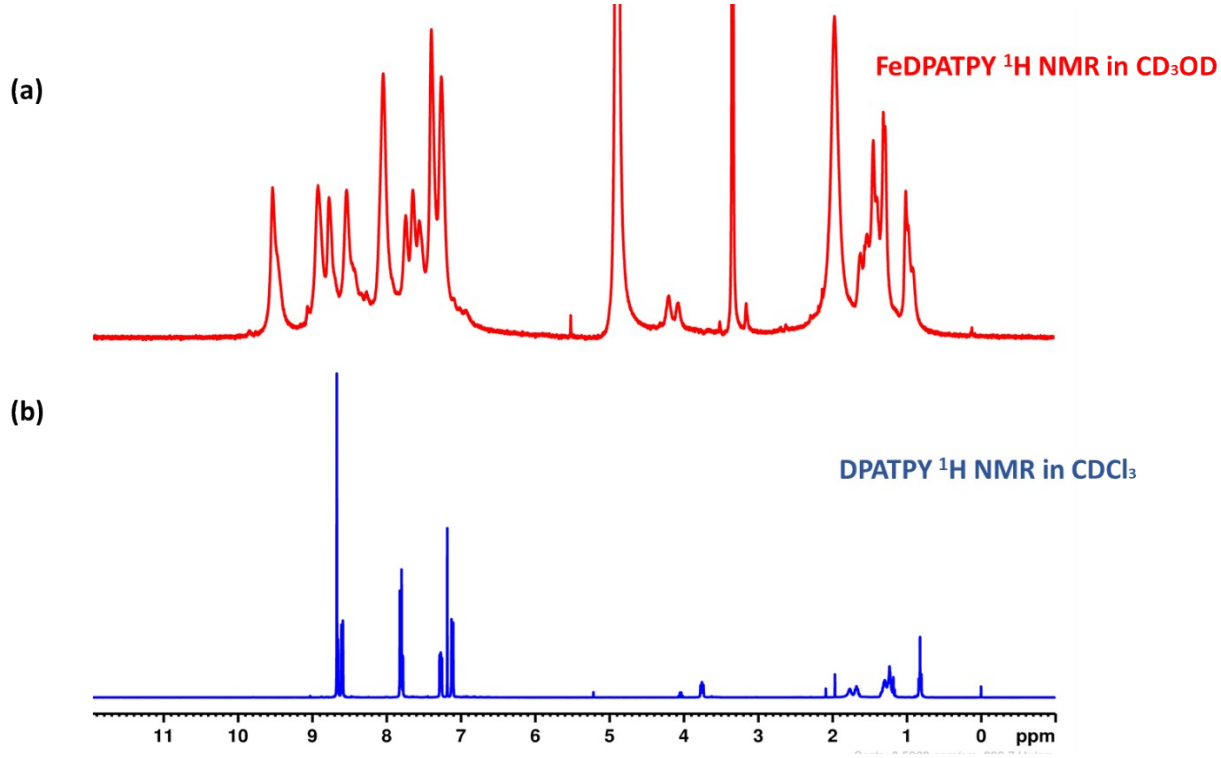

Fig. S12a: ^{1}H NMR spectrum of (a) **FeDPATPY** in CD_3OD (b) **DPATPY** in $CDCl_3$

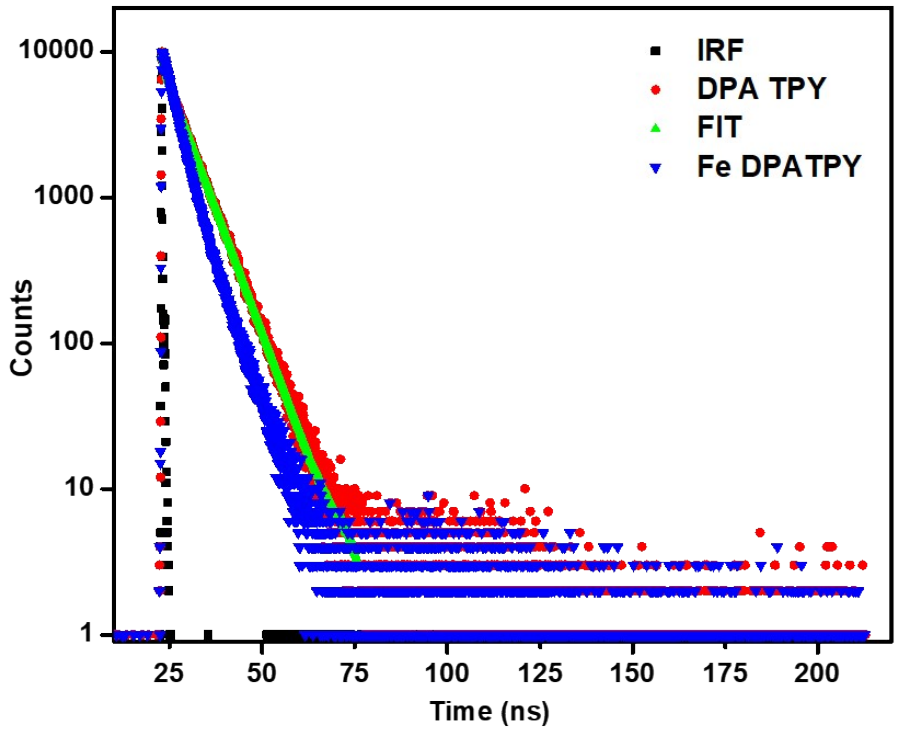

Fig. S13: Life Time decay profile of **DPATPY** and **FeDPATPY**

Table S1a: The lifetime parameters

Samples	α_1	α_2	α_3	τ_1	τ_2	τ_3	χ^2	τ (ns)

DPATPY	0.34	0.66	-	0.43	6.42	-	1.2	**6.22**
Fe DPATPY	0.13	0.71	0.16	0.16	3.34	6.81	1.0	**4.42**

Table S1b: Other fluorescence parameters

Samples	λ_{em} (nm)	Φ_f (%)	τ (ns)	k_r (10^6 s^{-1})	k_{nr} (10^8 s^{-1})
DPATPY	499	2.5	6.22	4.02	1.57
FeDPATPY	482	2.6	4.42	5.88	2.20

Where, λ_{em} = Emission maxima, Φ_f = relative quantum yield , τ = Fl. lifetime k_r = Radiative rate constant = Φ_f/τ, k_{nr} = Nonradiative rate constant = $(1/\tau)- k_r$

Table S2: All the crystallographic parameters of the ligand **DPATPY**

Compounds	**DPATPY**
Emp. formula	$C_{49}H_{43}N_7$
Formula weight	729.90
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	14.5275(2)
b/Å	8.93710(10)
c/Å	31.1191(5)
α/°	90
β/°	102.802(2)
γ/°	90
Volume/$Å^3$	3939.87(10)
Z	4
D_{calc}/g cm^3	1.231
μ/mm^{-1}	0.573
F (000)	1544.0
Data/restraints/parameters	8357/0/506
S	1.100
R1 [I>=2σ (I)]	R_1 = 0.0488, wR_2 = 0.1338
wR2 [all data]	R_1 = 0.0558, wR_2 = 0.1385
Max./min. residual electron dens. [e $Å^{-3}$]	0.23/-0.26

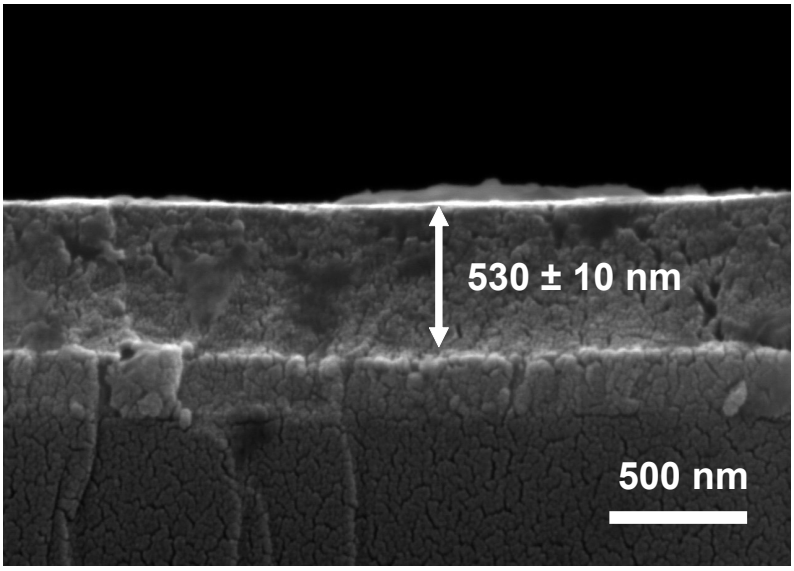

Fig. S14: Cross-sectional SEM image to derive the Fe-DPATPY film thickness on ITO-coated glass.

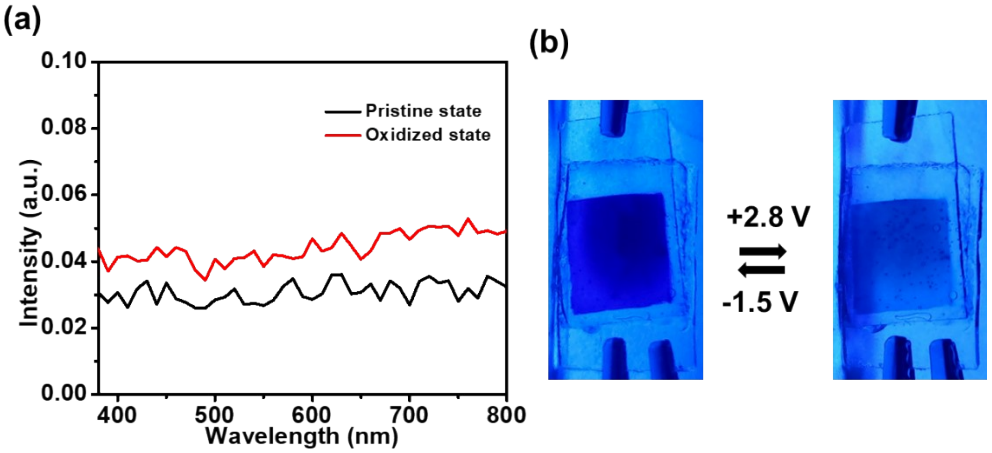

Fig. S15. (a) Emission spectra (excitation at 372 nm) and (b) the emission color change of the Fe-DPATPY-based ECD during the electrofluorochromism study. The photos are taken upon 365 nm UV-light irradiation.