

## **Supporting Information**

### **Design, Synthesis and Characterization of Novel Organic-Inorganic Hybrid Polymeric Materials for Electroluminescent Application**

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**1-Materials** Oxalyl Chloride, and Fe(II) acetate were purchased from Sigma Aldrich India and used without any further purification. Phthalic acid and sodium sulfite were purchased from SRL Pvt. Ltd. Celite, and sodium sulfate were purchased from HiMedia (India). 1,4-Dioxane and THF were purchased from SRL Pvt. Ltd and dried over sodium metal and benzophenone under a nitrogen atmosphere. All the solvents were AR grade and purified by standard procedure wherever required. All the reactions were carried out under dry nitrogen atmosphere.

**Caution:** Oxalyl Chloride is highly reactive and toxic when inhaled, so it should be handled with care and with proper precautions to avoid inhalation.

## **2-Instrumentations**

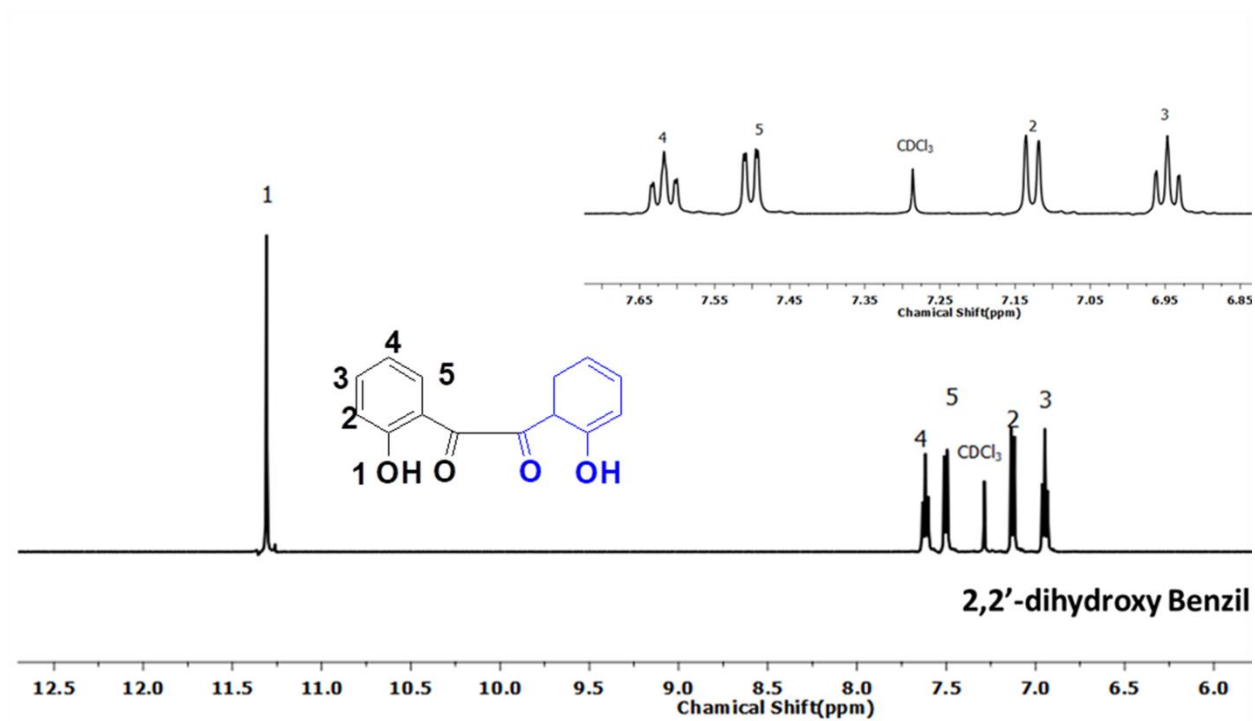
Bruker 400Hz was used for  $^1\text{H}$  NMR,  $^{13}\text{C}$  NMR Characterization with TMS as a reference. Perkin Elmer FT-IR C91158 spectrophotometer with zinc selenide crystal was used for ATR-IR (Attenuated total reflectance Infra-Red) spectra of ligand and polymers in the range of 4000-400  $\text{cm}^{-1}$ . The High-resolution mass spectra (ESI-HRMS) of ligand was recorded on Bruker daltronics microTOF-QII® spectrometer using ESI ionization. The Elemental analysis was done by CHNS Elementar Vario micro cube Analyzer. RIGAKU ULTIMA IV X-ray diffractometer was used for X-ray diffraction (WXRd) patterns between the range of  $2\theta=5-80^\circ$  at a scan rate of  $4^\circ/\text{min}$  using Ni filtered  $\text{CuK}\alpha$  as a radiation source. The UV measurements were measured on the UV spectrophotometer of Shimadzu. Cyclic voltammetry (CV) measurements were performed using cyclic voltammeter CH instruments, CH1620E at a scan rate of 100mV/sec. The absolute molecular weight of the polymer samples was recorded by the Static Light Scattering

experiment (SLS) in batch mode using Brookhaven BI-200SM goniometer using filtered stock solution and solvent through 0.2  $\mu$  Nylon filter.

### **3- Synthesis of Materials**

#### **3.1- Synthesis of 2,2'-dihydroxy Benzil (2)**

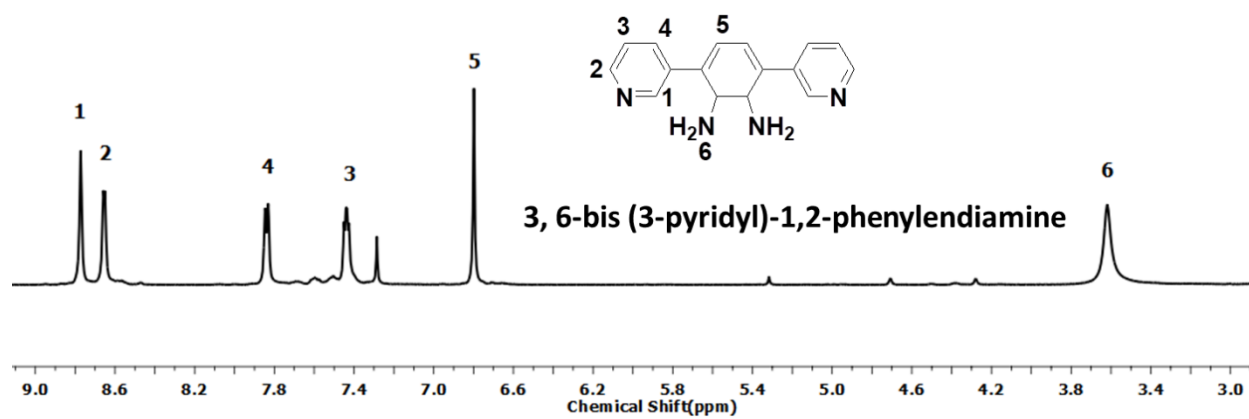
The Suspension of  $\text{AlCl}_3$  (11.20 g, 84.21 mmol) was made in 75 ml of  $\text{CH}_2\text{Cl}_2$  then a solution of phenol (3.95 gm, 42 mmol) in 15 ml  $\text{CH}_2\text{Cl}_2$  was added to it dropwise at RT and the mixture was stirred for 60 minutes. Another solution of Oxalyl Chloride (1.72 ml, 20 mmol) in 15 ml  $\text{CH}_2\text{Cl}_2$  was added dropwise, the reaction mixture was stirred for 4h at RT. After 4 h, the reaction was quenched by addition of 6 M HCl solution. The organic layer was separated and washed with water three times, dried over anhydrous  $\text{Na}_2\text{SO}_4$  and concentrated. The crude product was purified with column chromatography with  $\text{CH}_2\text{Cl}_2$  forming a yellow product that were crystallized with DCM:Hexane mixture Yield: 4.65 g (65 %).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 8.77 (s, 2H), 8.65 (d, 2H), 7.84 (d, 2H), 6.80 (s, 2H), 7.44 (t, 2H), 3.62 (s, 4H).



**Fig. S1.**  $^1\text{H}$ -NMR spectrum of 2,2'-dihydroxy Benzil in  $\text{CDCl}_3$

### 3.2 -Synthesis of 3, 6-Bis (3-pyridyl)-1, 2,-phenyldiamine (3)

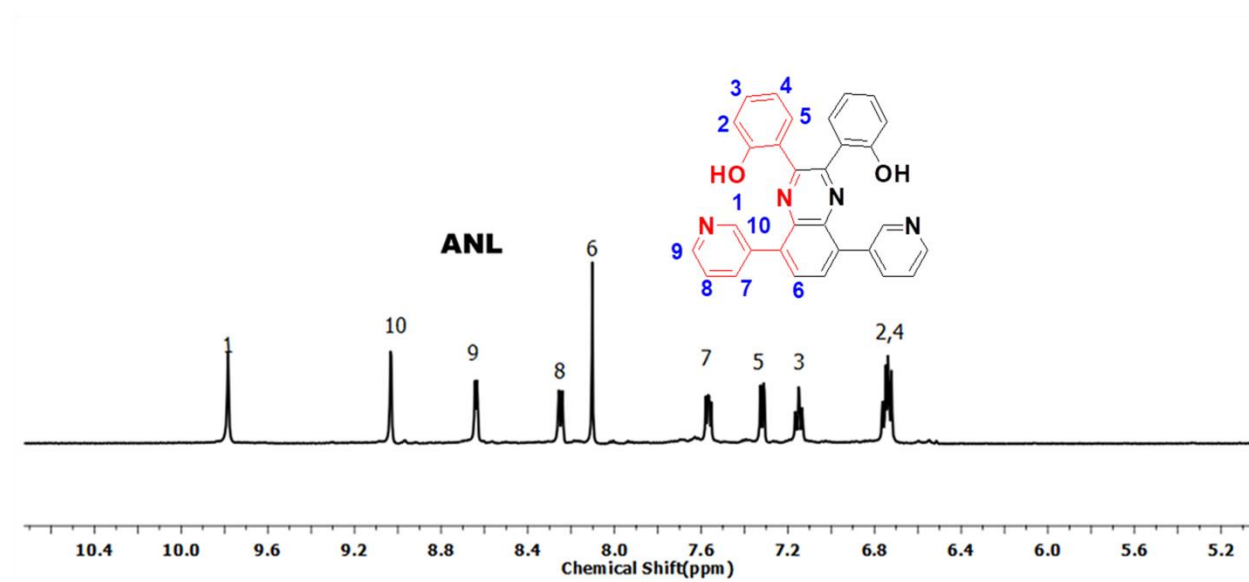
4, 7-Bis (3-pyridyl)-2, 1, 3-benzothiadiazole (1.00 g, 3.4 mmol),  $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$  (82 mg, 0.34 mmol), and  $\text{NaBH}_4$  (657 mg, 18.89 mmol) were added in a mixture of solvents Ethanol: THF (35:15). The black suspension was heated to reflux for 2h for  $80^\circ\text{C}$  after that reaction mixture was passed through Celite and the solvent was removed with rotary evaporator then the product was extracted by  $\text{CH}_2\text{Cl}_2$ , washed with brine solution, and dried over anhydrous  $\text{Na}_2\text{SO}_4$ , forming yellow solid Yield: 866 mg (96%).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 8.77 (s, 2H), 8.65 (d, 2H), 7.84 (d, 2H), 6.80 (s, 2H), 7.44 (t, 2H), 3.62 (s, 4H).



**Fig. S2.**  $^1\text{H}$ -NMR spectrum of 3, 6-bis (3-pyridyl)-1,2-phenyldiamine in  $\text{CDCl}_3$

## 4-Characterization

### 4.1- $^1\text{H}$ NMR spectrum of ANL



**Fig. S3.**  $^1\text{H}$ -NMR spectrum of ANL in  $\text{DMSO-d}_6$

#### 4.2- $^{13}\text{C}$ NMR spectrum of ANL

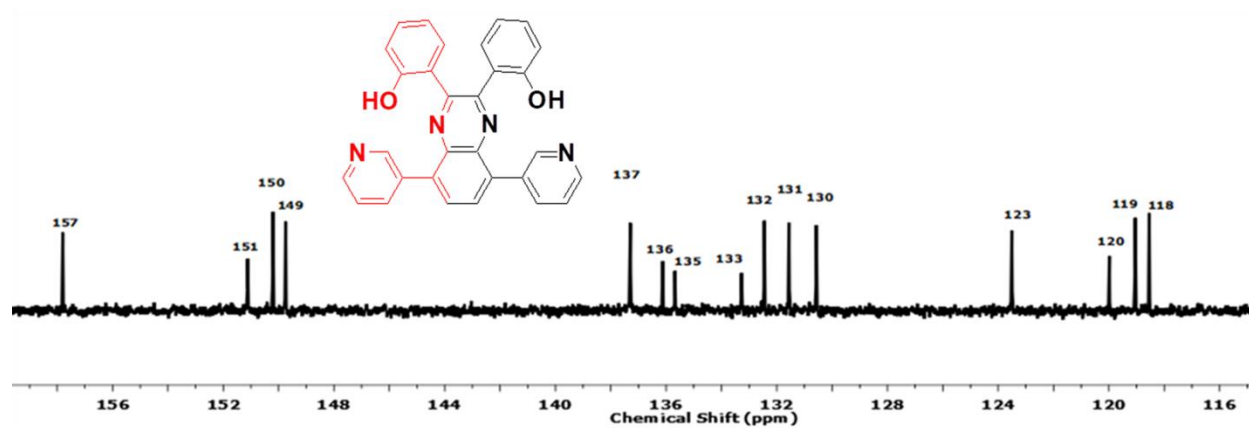
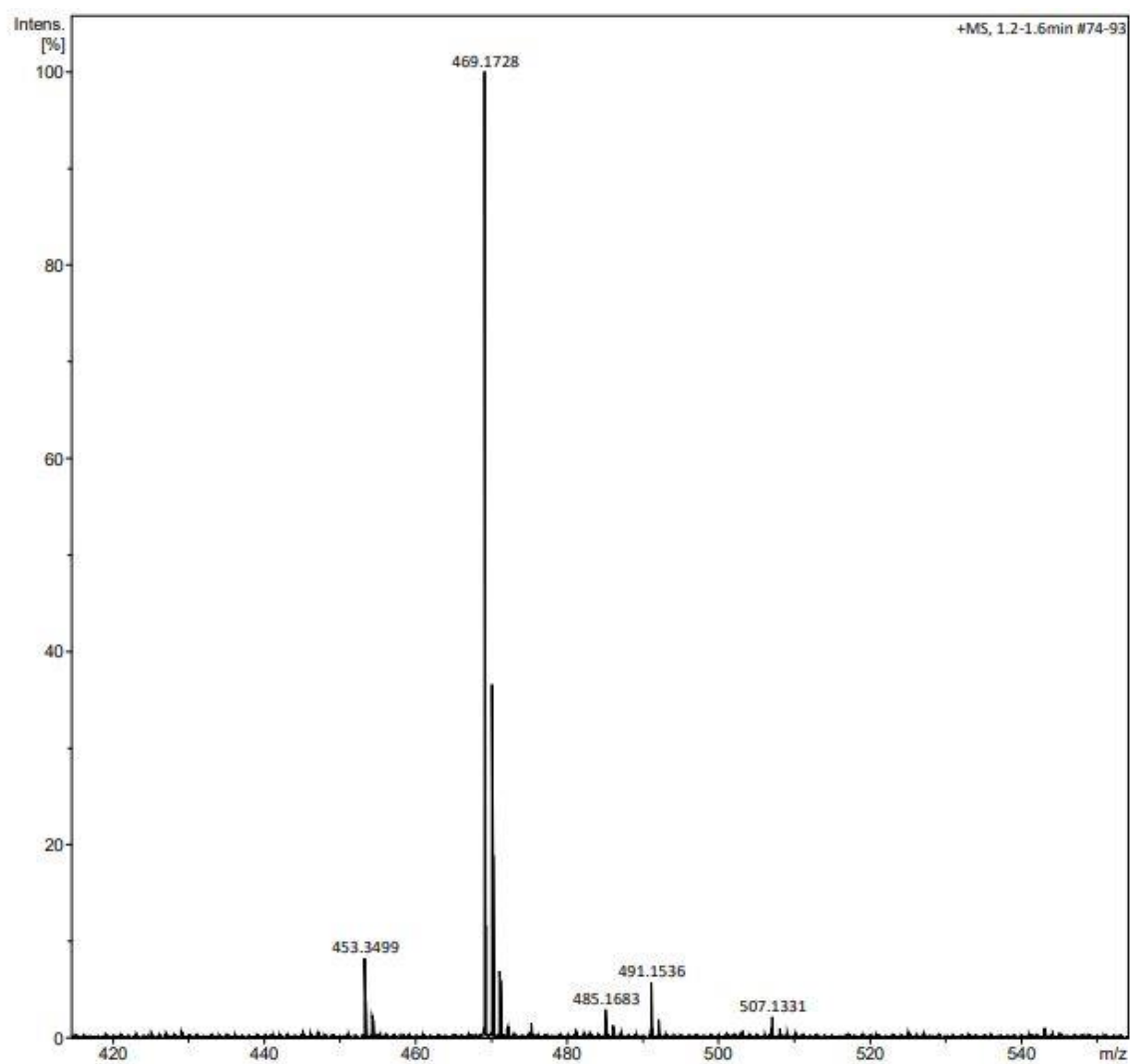


Fig. S4.  $^{13}\text{C}$ -NMR spectrum of ANL (4) in  $\text{DMSO-d}_6$

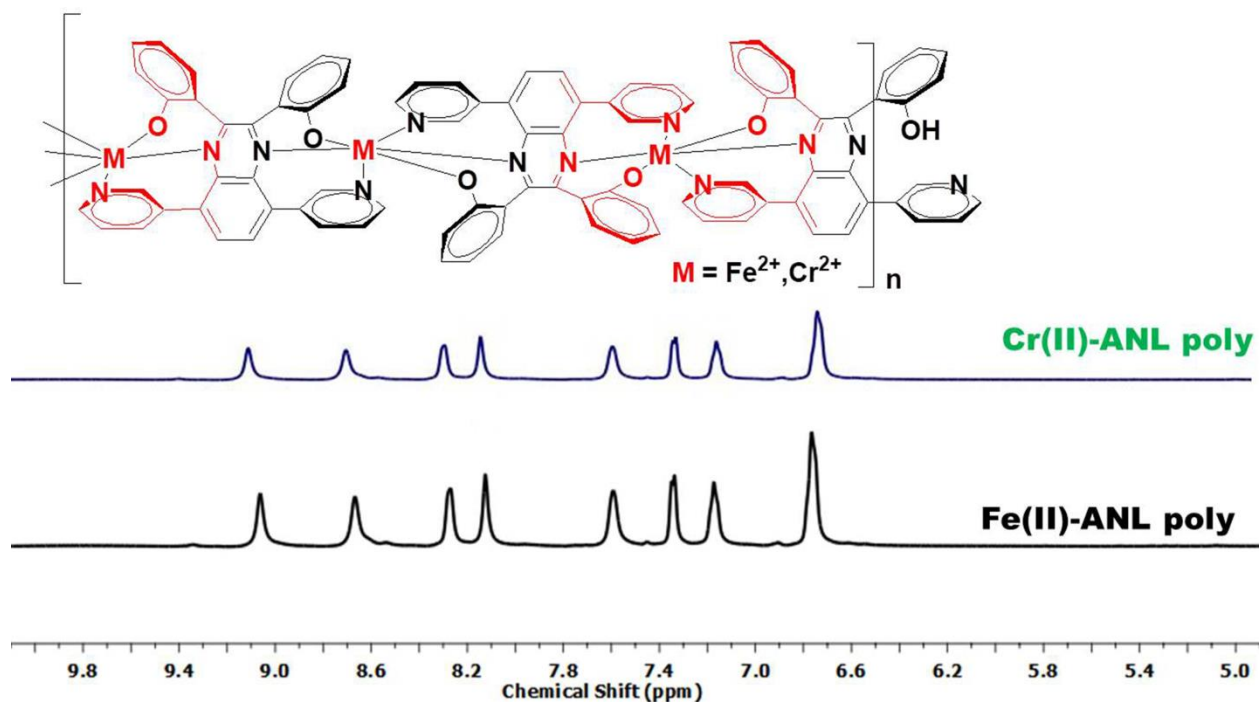
#### 4.3-MS (HRMS-ESI) of ANL

Calculated for  $C_{30}H_{20}N_4O_2$  (m/z): 468.0523 and found: 469.1728. ( $M+H^+$ )



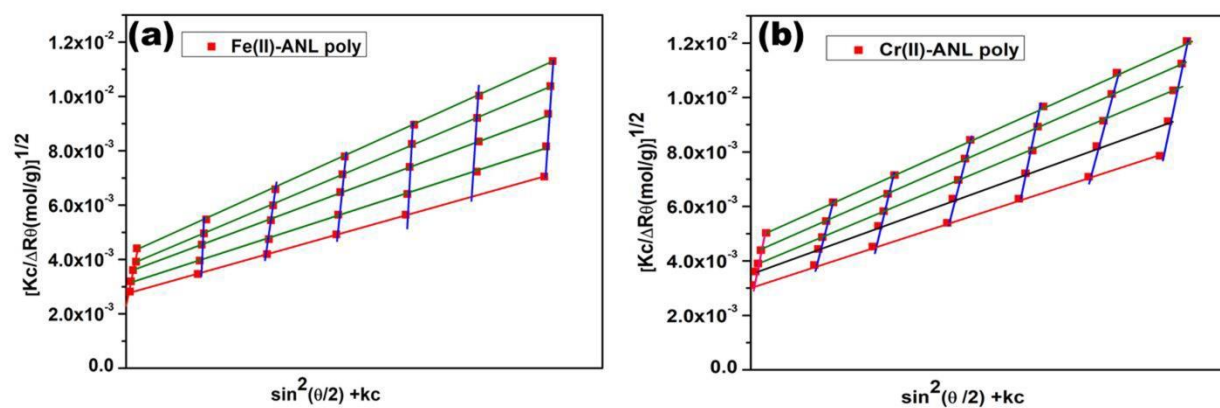
**Fig. S5.** HRMS Spectra of ANL

#### 4.4- $^1\text{H}$ NMR spectra of Fe(II)-ANL poly and Cr(II)-ANL poly



**Fig. S6.**  $^1\text{H}$ -NMR spectrum of Fe(II)-ANL poly and Cr(II)-ANL poly in  $\text{DMSO-d}_6$

#### 4.5-Molecular Weight Determination of Fe(II)-ANL poly and Cr(II)-ANL poly by SLS



**Fig. S7.** Berry Plot of (a) Fe(II)-ANL poly, and (b) Cr(II)-ANL poly in batch mode in THF solution

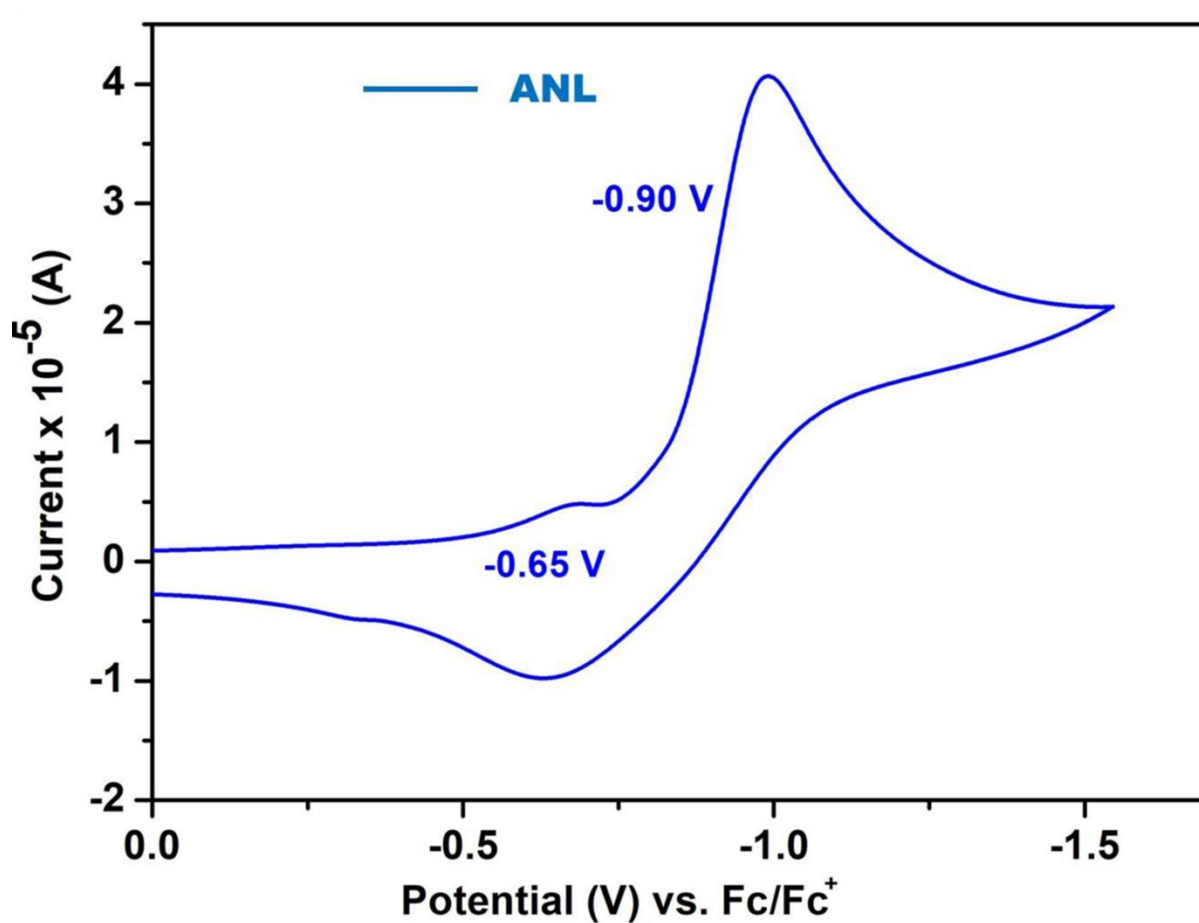


**4.6- Table-1- Conductivity Measurement of Fe(II)-ANL poly and Cr(II)-ANL poly solutions in Methanol**

Sr No.	Concentration	Ionic NaCl (Conductivity) ( $\mu\text{S}$ )	Metal Salts $\text{Fe}(\text{OAc})_2$ (Conductivity) ( $\mu\text{S}$ )	Covalent Glucose (Conductivity) ( $\mu\text{S}$ )	Fe(II)-ANL poly (Conductivity) ( $\mu\text{S}$ )	Cr(II)-ANL poly (Conductivity) ( $\mu\text{S}$ )
1	$10^{-2}$	738	106	2.08	28.17	40.24
2	$10^{-3}$	78.40	44.40	1.54	27.04	38.55
3	$10^{-4}$	11.10	11.40	1.10	26.56	39.03

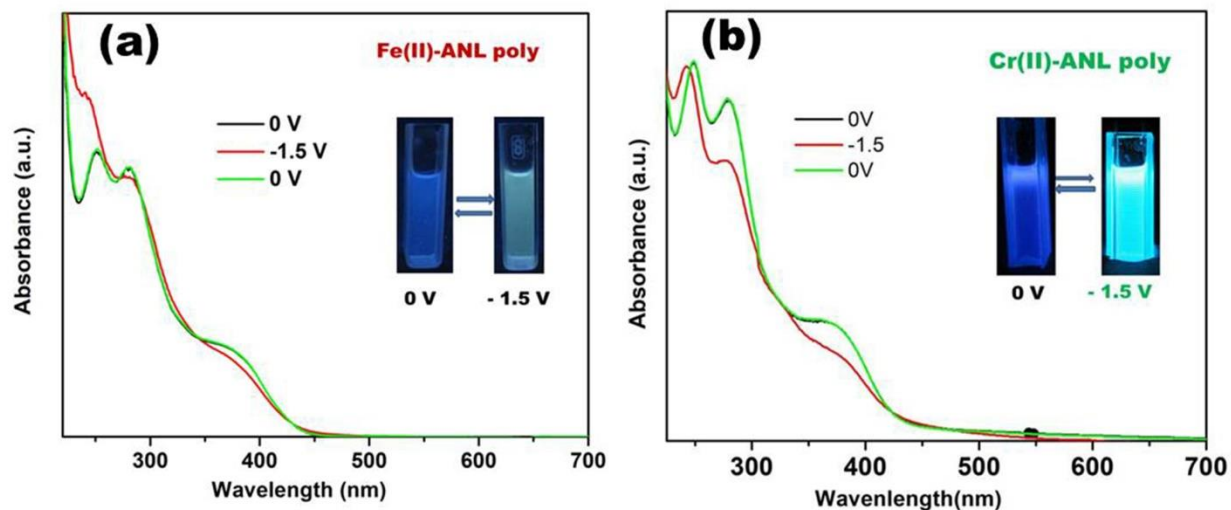
Measured conductivity of Methanol under the experimental condition at  $27^\circ\text{C}$  =  $1.54 \mu\text{S}$

#### 4.7- Cyclic Voltammogram of ANL



**Fig. S8.** Cyclic Voltammogram of ANL and Fe(II)-ANL poly in DCM

#### 4.8- Reversible Spectroelectrochemical measurement of Fe(II)-ANL poly and Cr(II)-ANL poly



**Fig .S9.** Reversible Spectroelectrochemical spectra of (a) Fe(II)-ANL poly, and (b) Cr(II)-ANL poly in DCM

The solution state Spectroelectrochemical experiment of Fe(II)-ANL poly and Cr(II)-ANL poly were carried out in a potential range of 0 V to -1.5 V. The change was observed on applying -1.5 V while upon the application of the reverse potential (0 V), the original spectrum was recovered.

#### References

- [1] R. Cavitands, I. Pochorovski, J. Milic, C. Gropp and W.B. Schweizer, J. Am. Chem. Soc. 2014, **136**, 3852–3858.
- [2] M.S. Seo, A. Lee and H. Kim, Org. Lett. 2014, **16**, 2950–2953.