

Supplementary information - Figures

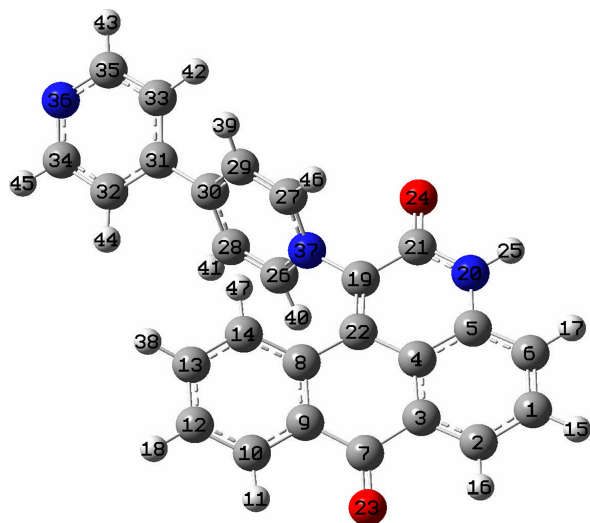


Figure S1-1

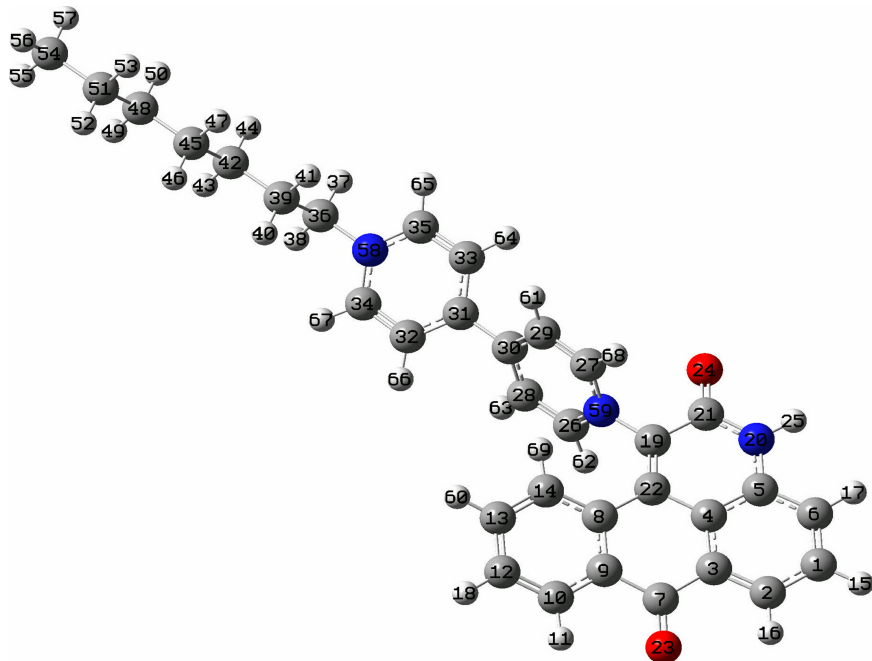


Figure S 1-2

Fig. S1 Optimized geometries of *1* (S1-1) and *2* (S1-2) at B3LYP/6-311++G** level acetonitrile with serial number of atoms using Gaussian 03W software

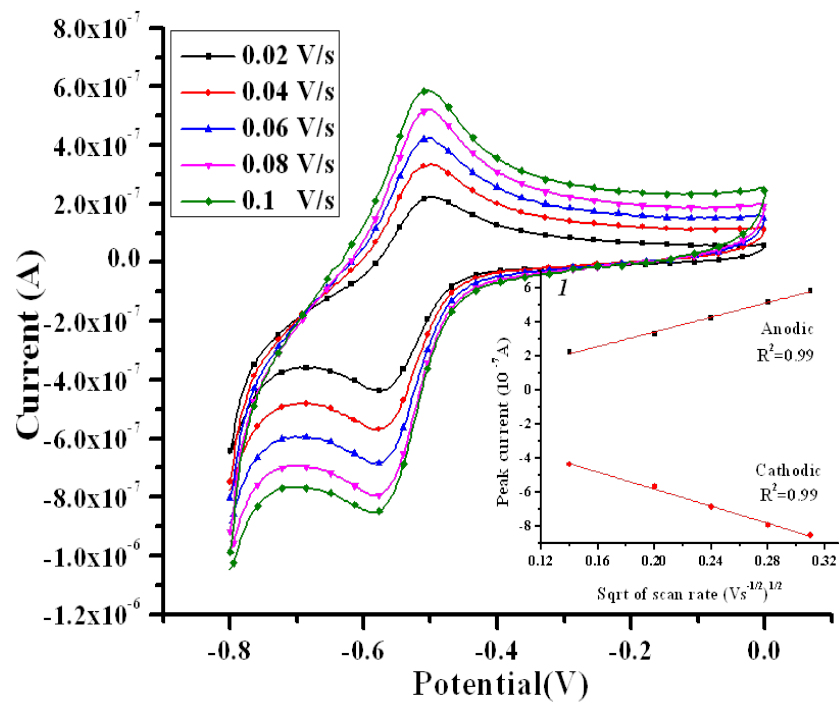


Figure S2a

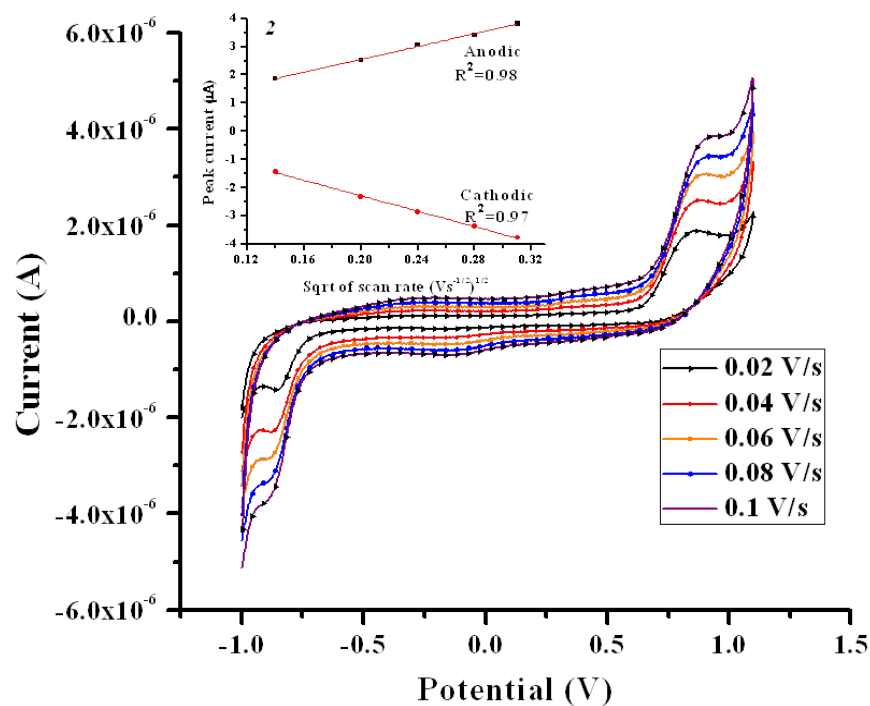


Figure S2b

Fig. S2 Cyclic voltammograms of **1**(S2a) and **2**(S2b) (10^{-4} M) in acetonitrile (ACN) at different scan rates 20, 40, 60, 80, 100mVs $^{-1}$ using 0.1M TBAP as supporting electrolyte and GC as working electrode

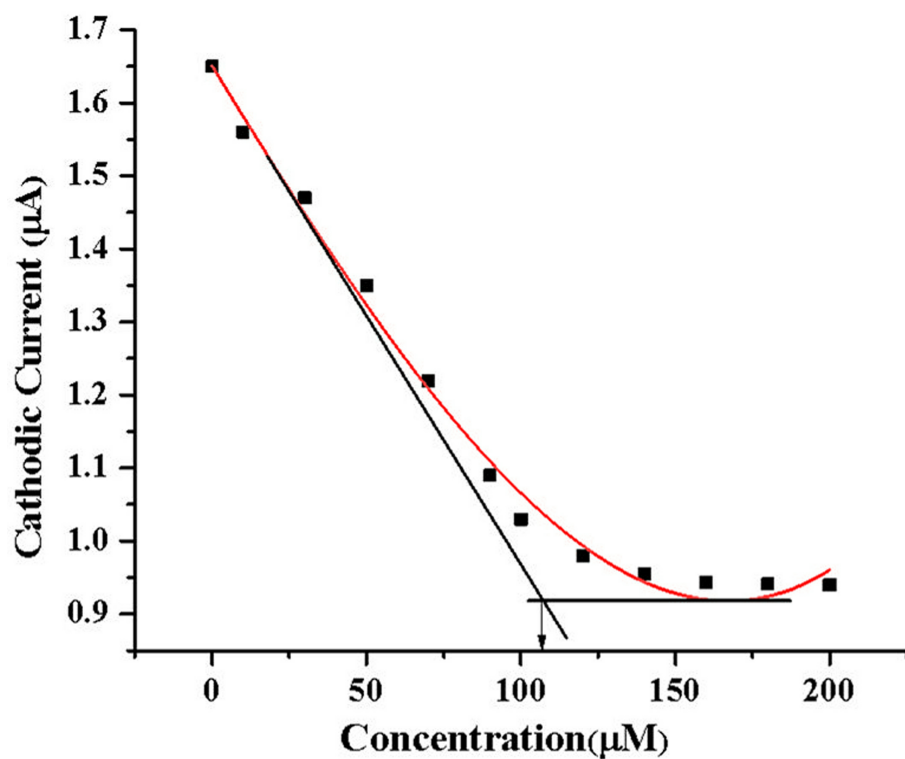


Figure S4

Fig. S4 Calibration plots between concentration of cyanide and current in acetonitrile medium using 0.1M TBAP as supporting electrolyte (GC working electrode, scan rate 20 mVs^{-1} E vs Ag/Ag^+)

Tables

Table S1. Energies of HOMO and LUMO for molecules *1* and *2* measured using Gaussian 03W software

Molecule	Energy in eV				
	E _{HOMO}	E _{LUMO}	E _{LUMO+1}	E _{gap1}	E _{gap2}
<i>1</i>	-9.1948	-0.3221	-0.0933	8.8727	9.1015
<i>2</i>	-7.0157	-3.655	-3.2947	3.3607	3.721

$E_{\text{gap1}} = E_{\text{LUMO}} - E_{\text{HOMO}}$, $E_{\text{gap2}} = E_{\text{LUMO+1}} - E_{\text{HOMO}}$

Table S2. Cathodic shift in peak potential (with binding constants) of *1* and *2* on interaction with different anions

Anions (2equivalents)	<i>1</i>		<i>2</i>
	$\Delta E_{\text{pc}}(\text{mV})$	Binding constant(M ⁻¹)	$\Delta E_{\text{pc}}(\text{mV})$
Cyanide	∞	∞	∞
Acetate	115	74	-
Fluoride	106	53	-
Chloride	13	1.4	9
Bromide	1	1.3	9
Iodide	1	1.3	7
Hydrogen sulphate	15	1.4	1

ΔE_{pc} shift in cathodic peak potential