Supporting information

Diphenylether based derivatives as Fe (III) chemosensors: Spectrofluorimetry, Electrochemical and Theoretical studies

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Table S1: Comparison of chemosensors used for detection of Fe^{3+} by various techniques

S. No.	Receptors	Technique used	Interference	Linear range	Reference
1	2-amino-6-methyl-4-phenyl-nicotinonitrile	Fluorescence	Hg^{2+}	2×10^{-4} to 7×10^{-4}M	42
2	Aminobisulfonate receptor	Fluorescence	Cu^{2+}	16×10^{-6} to 63×10^{-6} M	7
3	Diphenylfluorenes	UV, Fluorescence	Co^{2+}	1×10^{-6} to 8×10^{-6} M	3
4	Dimethyliminocinnamyl linked rhodamine	Voltammetry	NA	1.0×10^{-1} to 1.0×10^{-5}M	43
5	Terpyridine based	UV, Colorimetry	Ag^{+}	2.0×10^{-5} to 8.0×10^{-5}M	44
6	**Proposed chemosensor**	UV, Fluorescence, CV, DPV	No interference	1×10^{-6} to 2.5×10^{-6} M	**Present work**

Table S2 Binding energies between **DPE** molecules and Fe^{3+}

Receptor	Energy in a.u
DPE-I	-1175
DPE-I+Fe^{3+}	-1298
DPE-II	-1177
DPE-II+Fe^{3+}	-1299

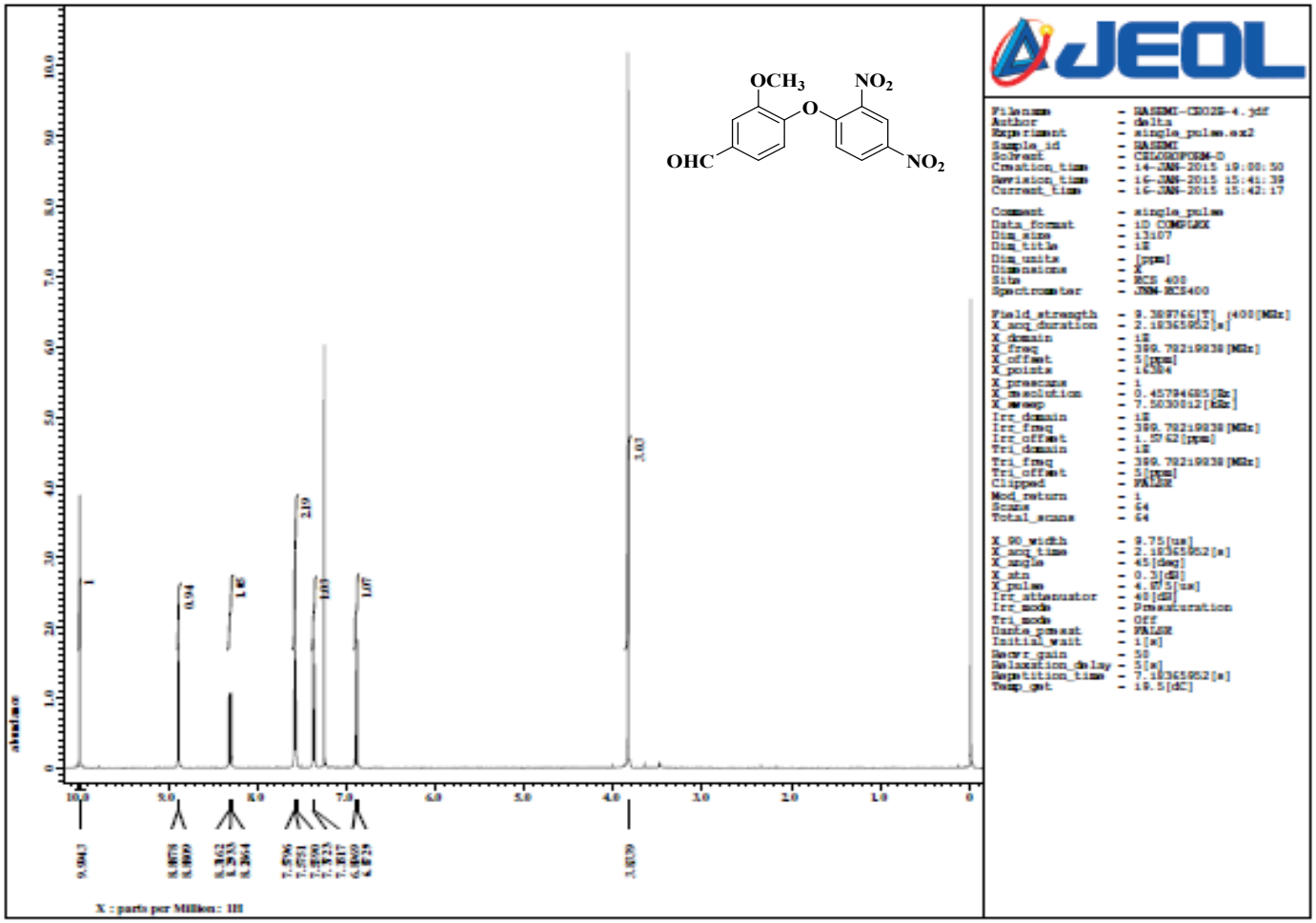


Figure S1 (a) ^{1}H NMR spectra of **DPE-I.**

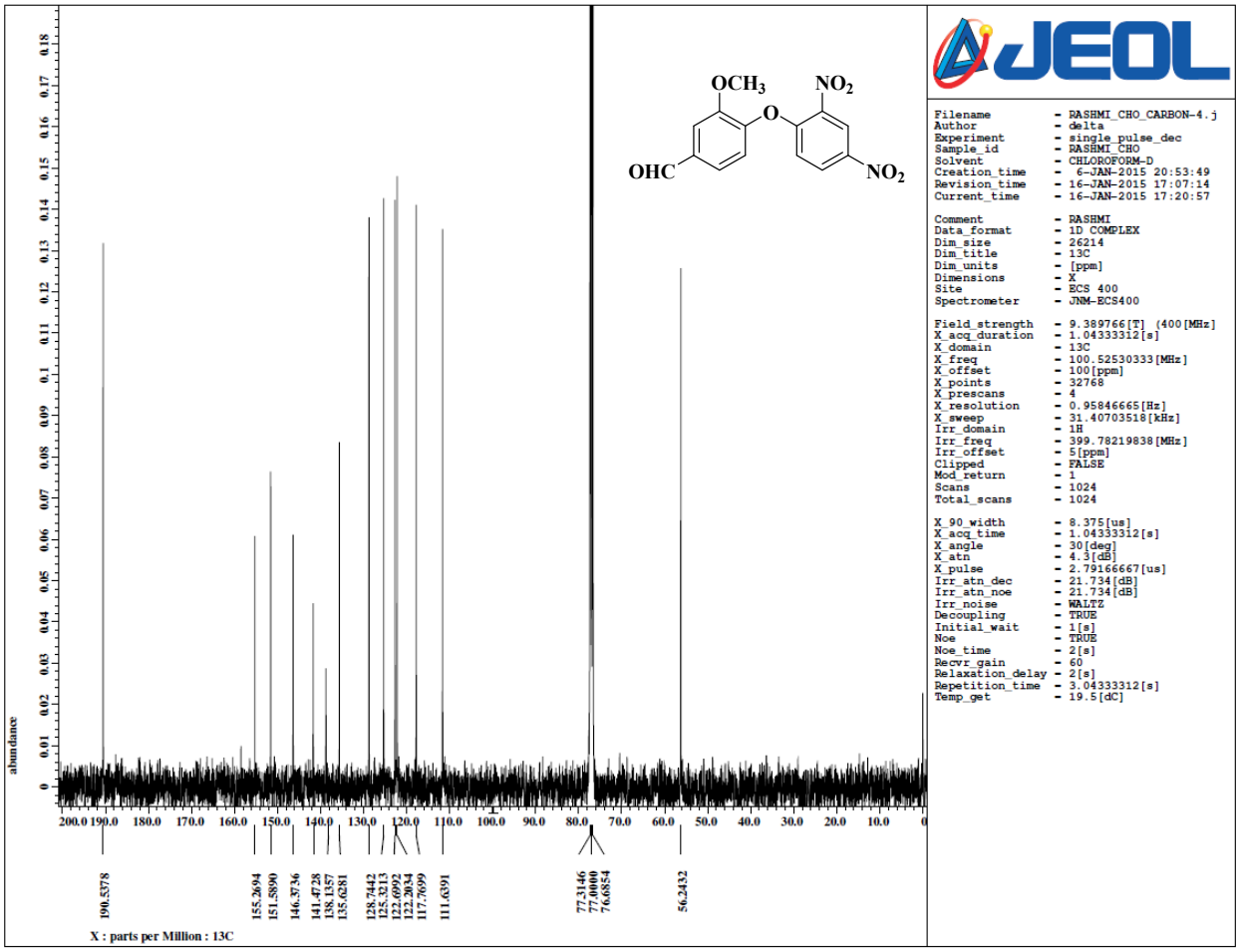


Figure S1 (b) ^{13}C NMR spectra of **DPE-I.**

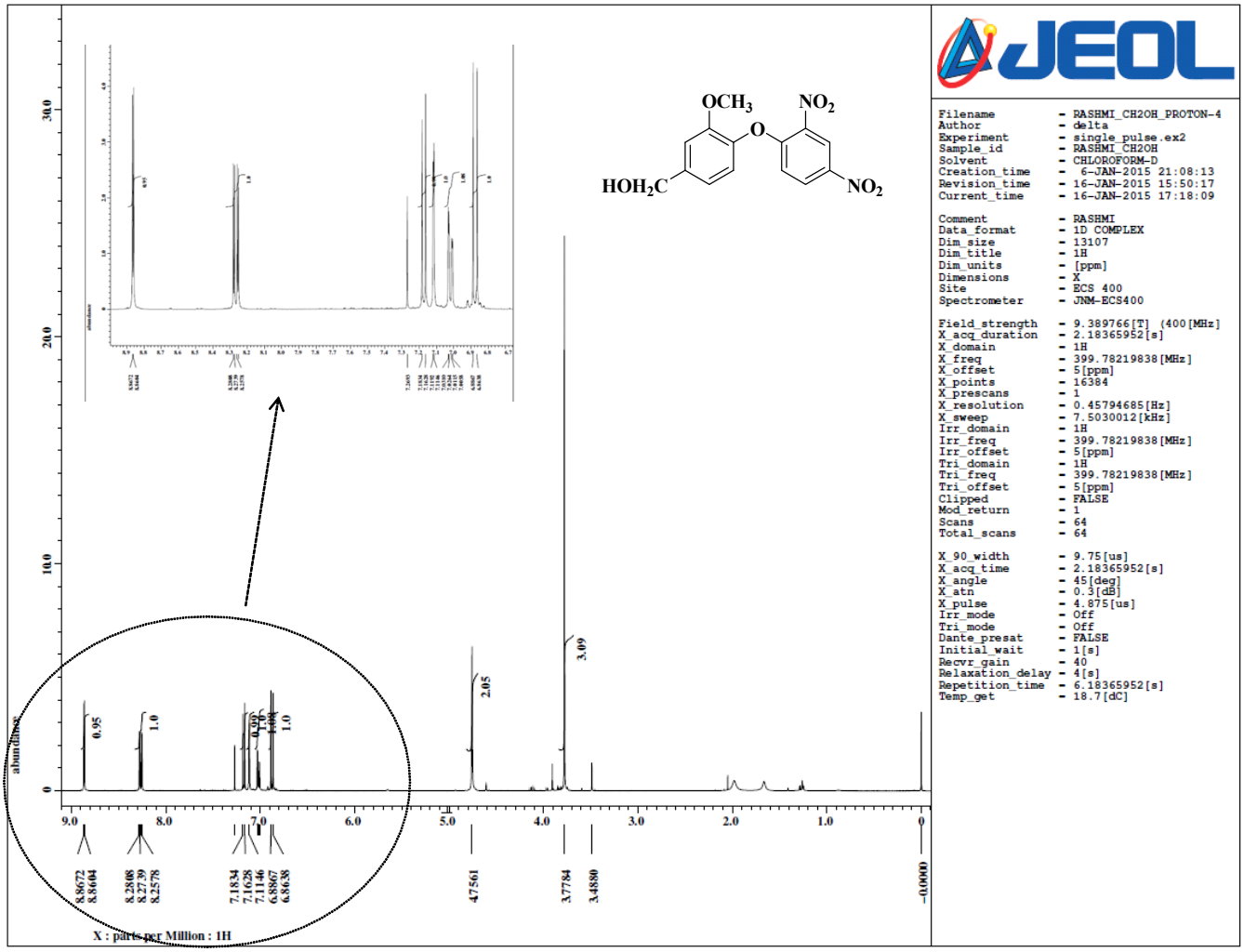


Figure S2 (a) ^{1}H NMR spectra of **DPE-II.**

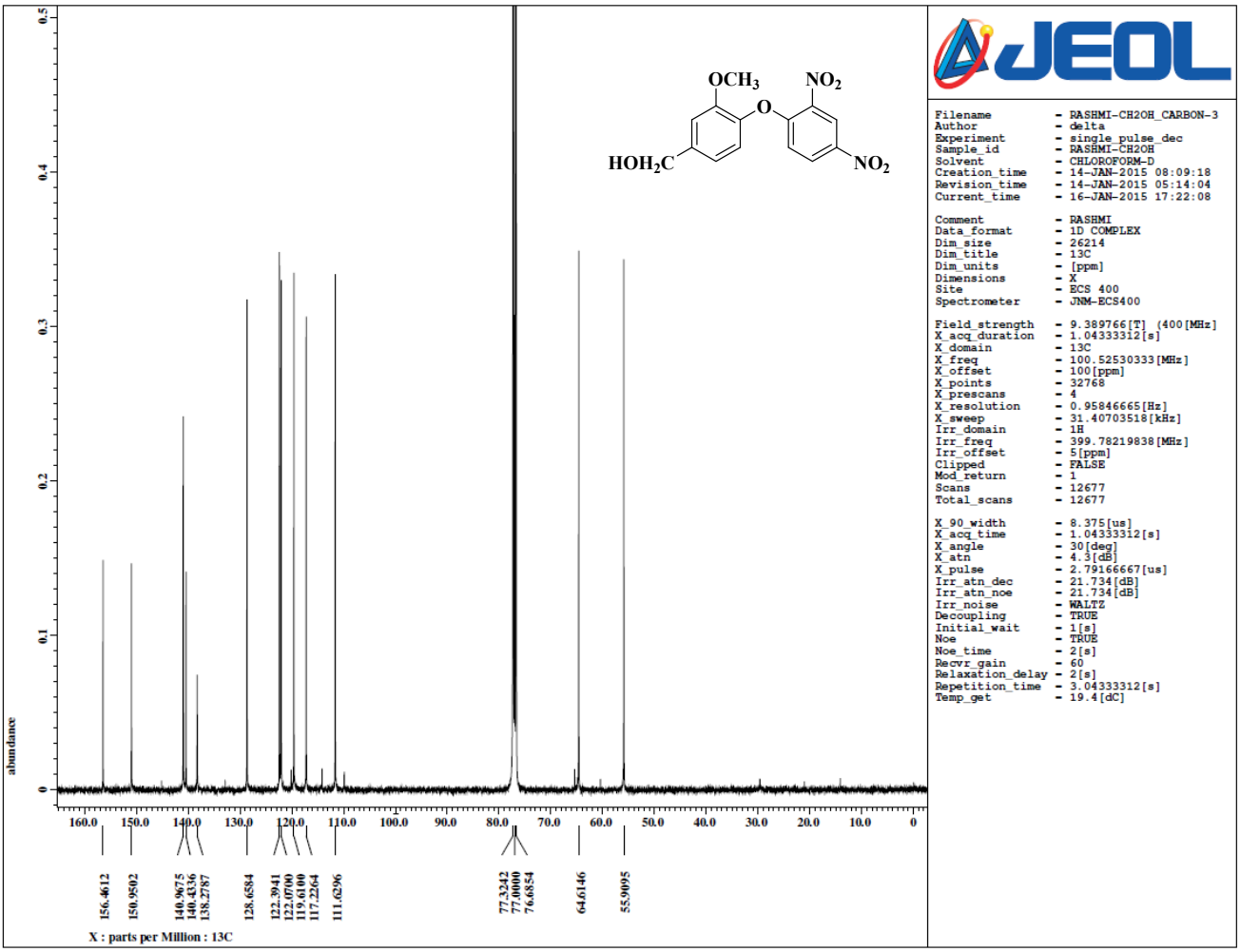


Figure S1 (b) ^{13}C NMR spectra of **DPE-II.**

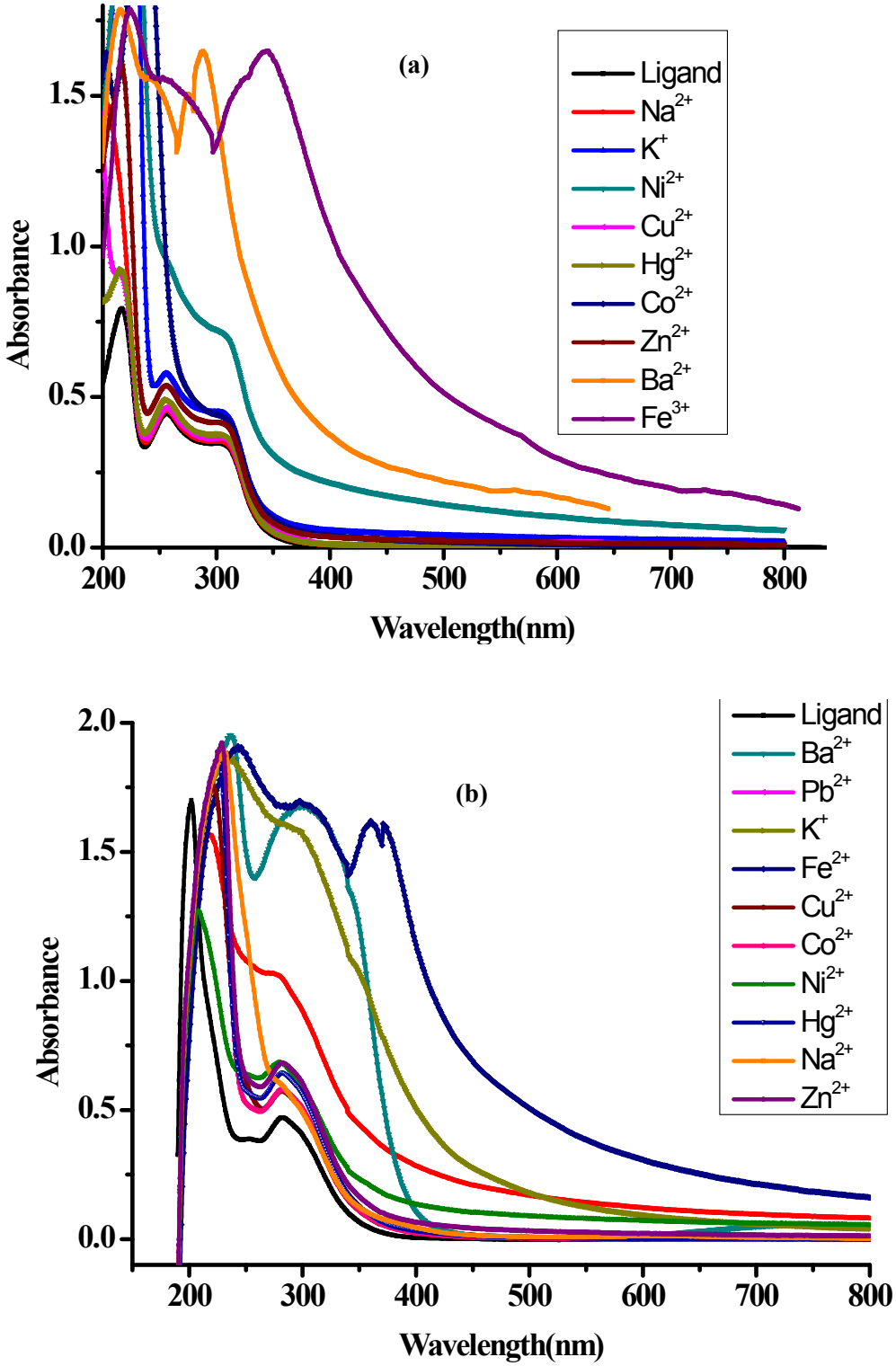


Figure S3 UV-Visible absorption spectra of (a) **DPE-I** (20 μM) and (b) **DPE-II** (20 μM) upon addition of a particular metal salt in HEPES buffered ACN/H_2O (9:1, v/v) solvent system.

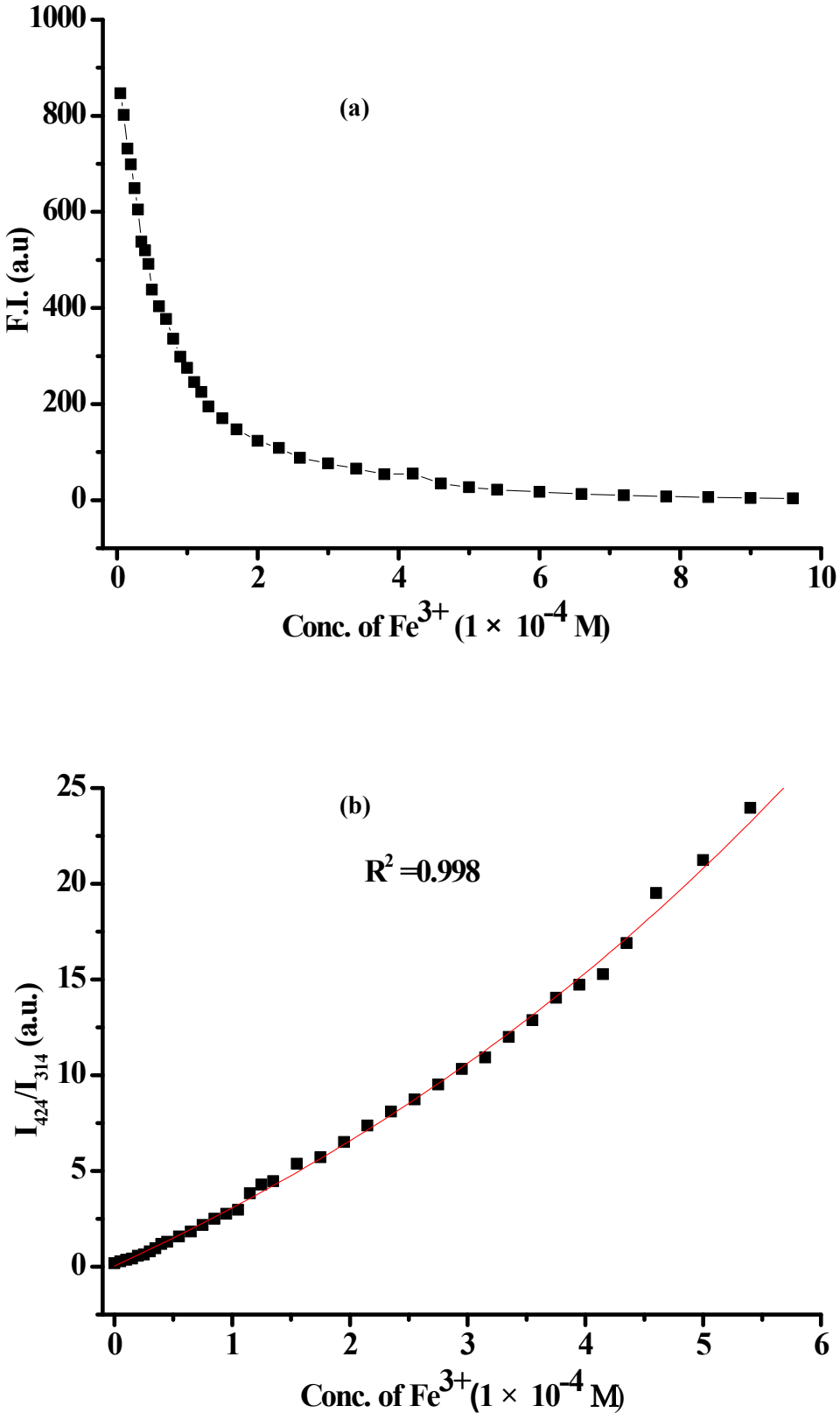
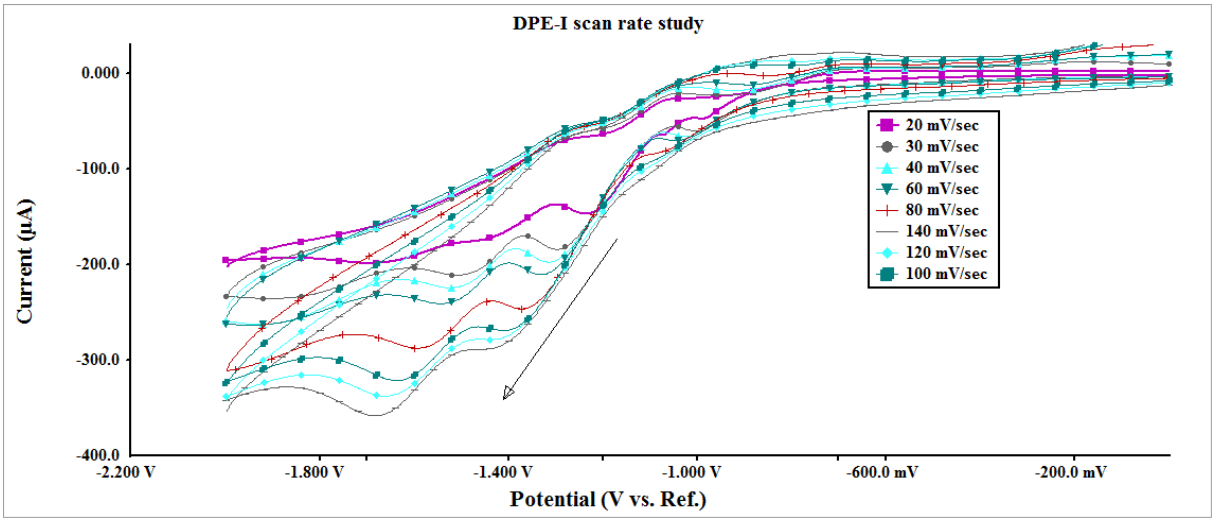
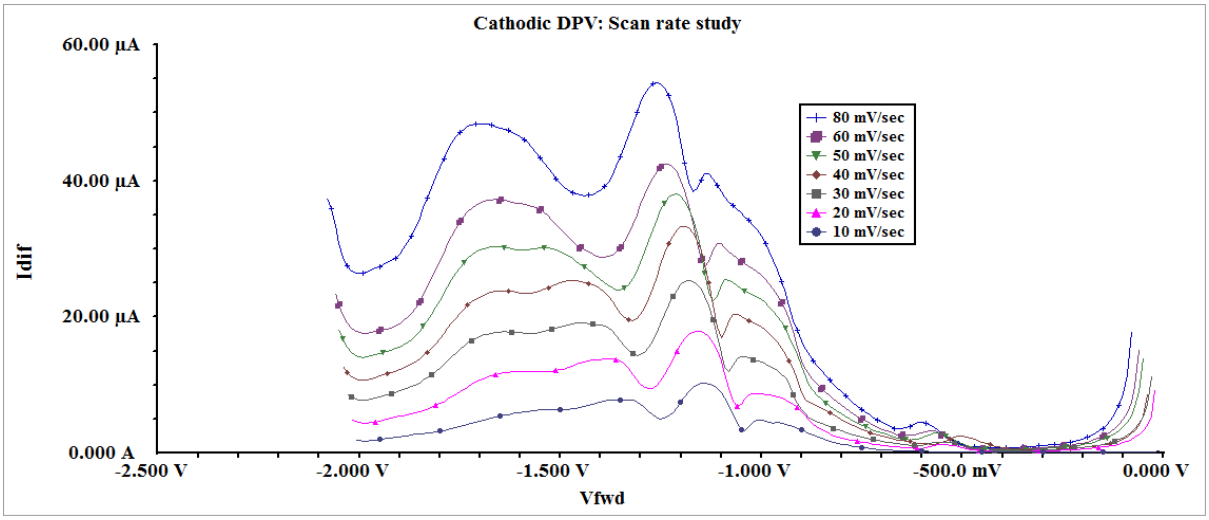


Figure S4 Ratiometric behavior of (a) **DPE-I** (b) **DPE-II** in presence of various Fe^{3+} ions conc. in HEPES buffered ACN/H_2O (9:1, v/v) solvent system.


DPE-I scan rate study
0.000
-100.0
-200.0
-300.0
-400.0
Current (µA)
-2.200 V
-1.800 V
-1.400 V
-1.000 V
-600.0 mV
-200.0 mV
Potential (V vs. Ref.)
20 mV/sec
30 mV/sec
40 mV/sec
60 mV/sec
80 mV/sec
140 mV/sec
120 mV/sec
100 mV/sec


Cathodic DPV: Scan rate study
60.00 µA
40.00 µA
20.00 µA
0.000 A
Idif
-2.500 V
-2.000 V
-1.500 V
-1.000 V
-500.0 mV
0.000 V
Vfwd
80 mV/sec
60 mV/sec
50 mV/sec
40 mV/sec
30 mV/sec
20 mV/sec
10 mV/sec

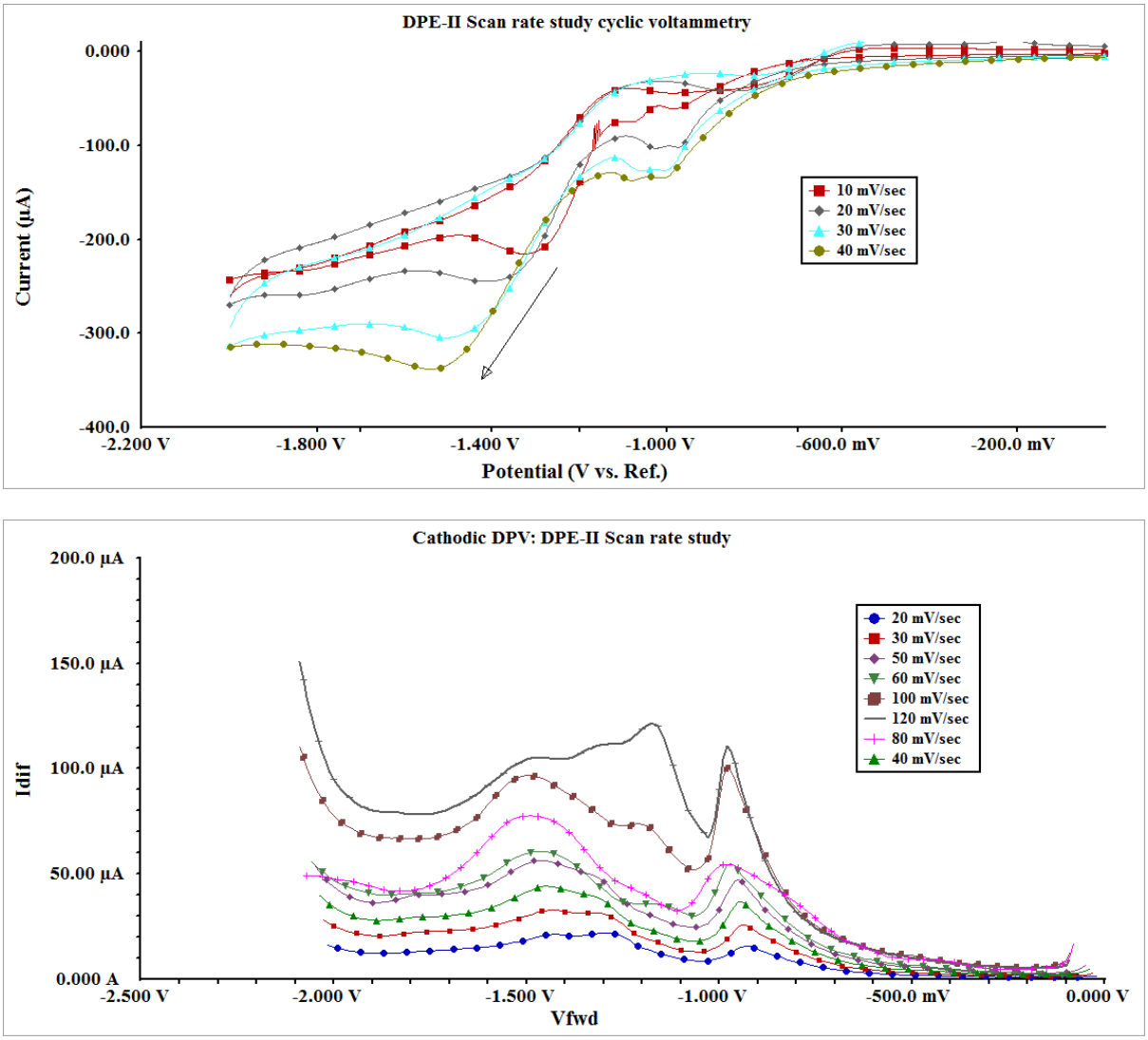
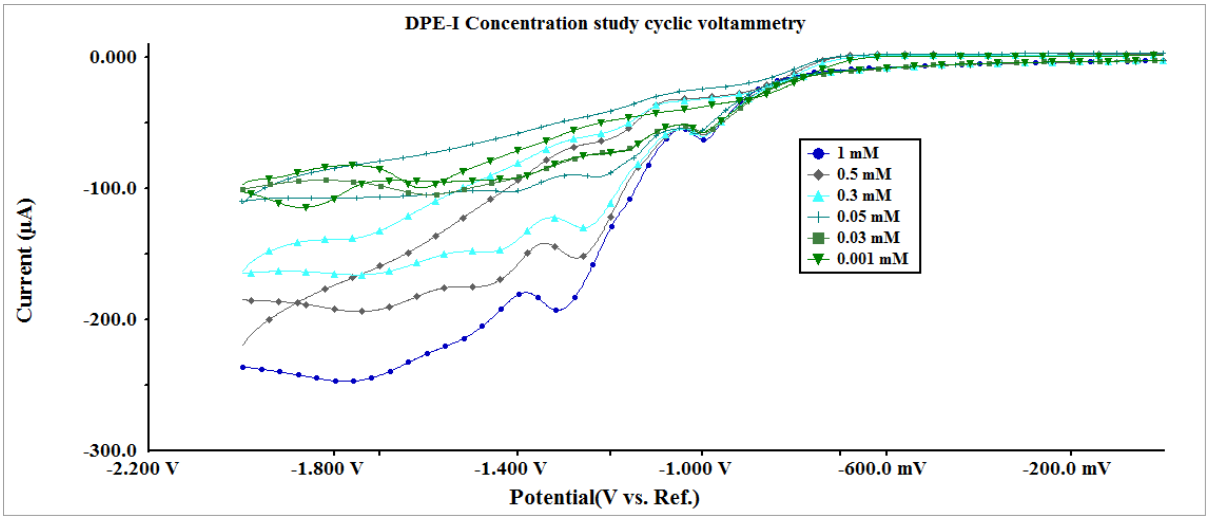


Figure S5 CV and DPV graphs of **DPE-I** and **DPE-II** with increase in scan rate in HEPES buffered ACN/H_2O (9:1, v/v) solvent system.



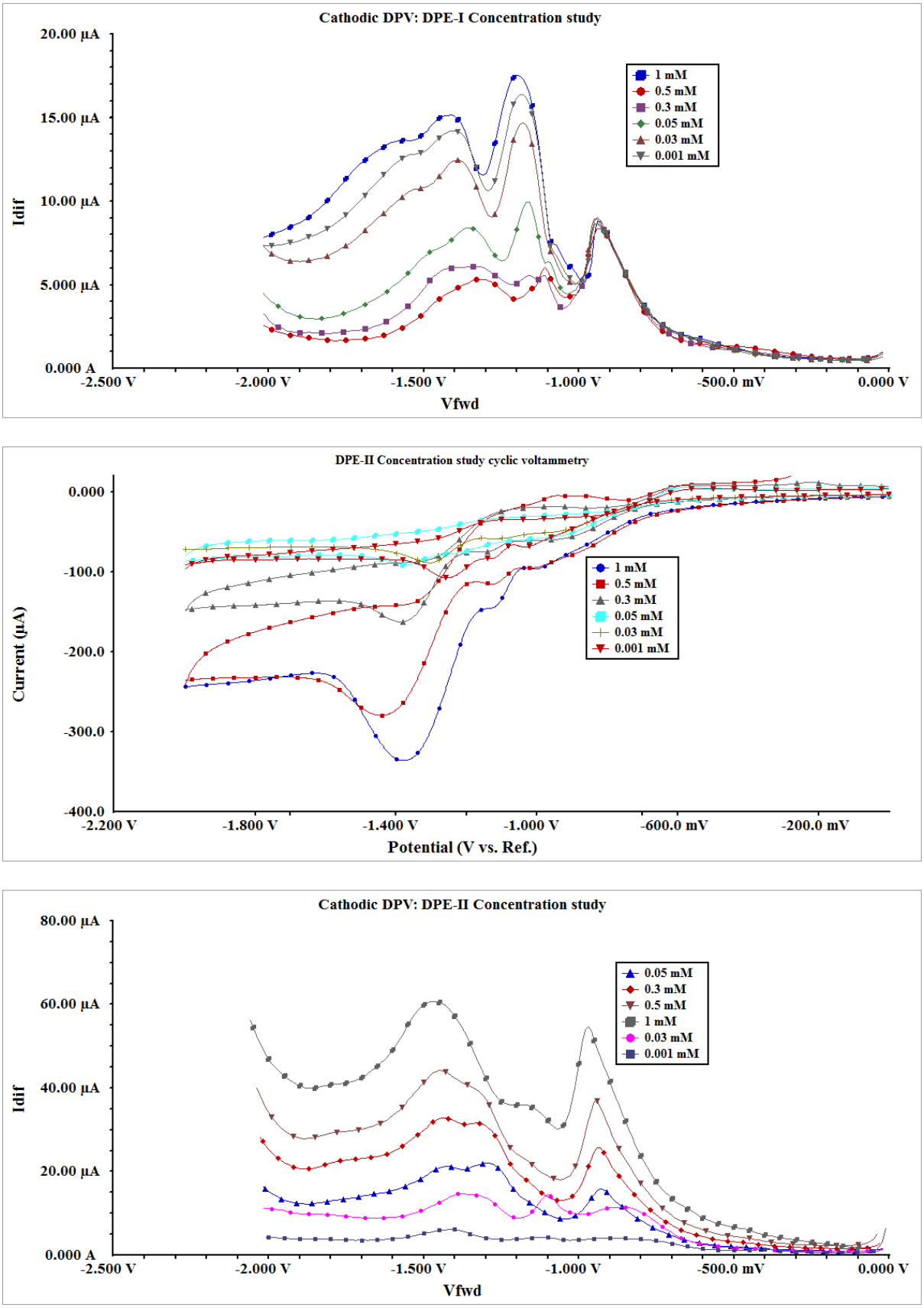
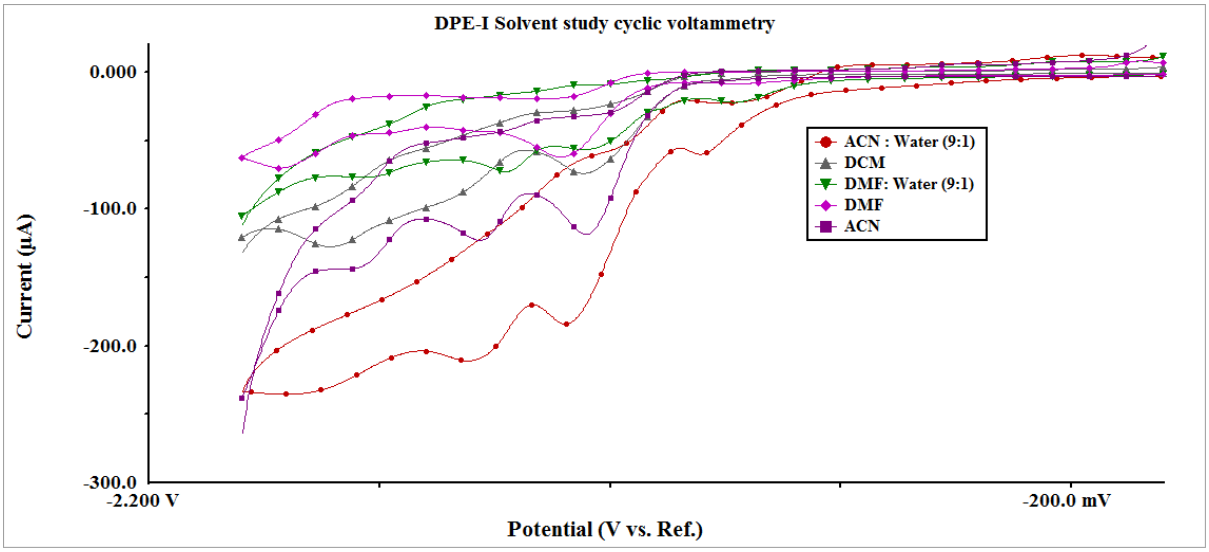
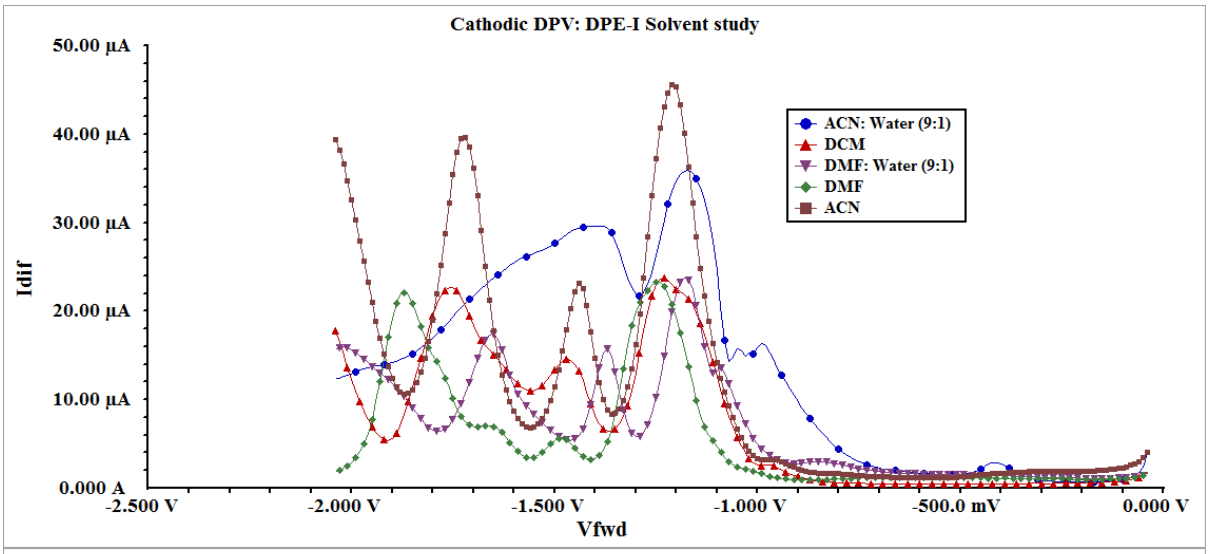
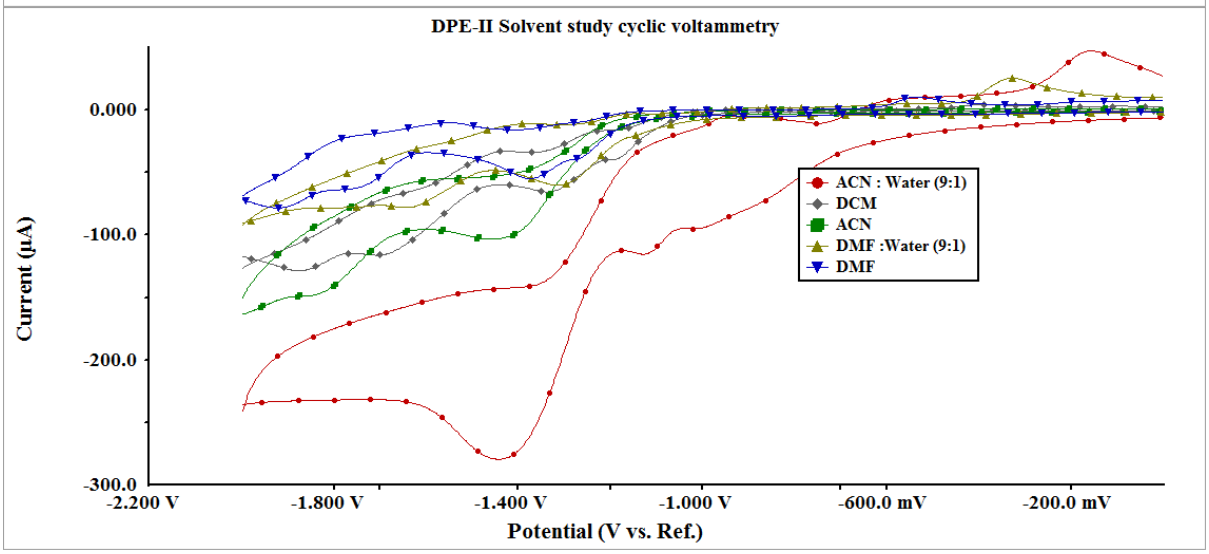


Figure S6 CV and DPV graphs of **DPE-I** and **DPE-II** with various concentrations of active species in HEPES buffered ACN/H_2O (9:1, v/v) solvent system.


DPE-I Solvent study cyclic voltammetry
0.000
-100.0
-200.0
-300.0
Current (µA)
-2.200 V
-200.0 mV
Potential (V vs. Ref.)
ACN : Water (9:1)
DCM
DMF: Water (9:1)
DMF
ACN


Cathodic DPV: DPE-I Solvent study
50.00 µA
40.00 µA
30.00 µA
20.00 µA
10.00 µA
0.000 A
Idif
-2.500 V
-2.000 V
-1.500 V
-1.000 V
-500.0 mV
0.000 V
Vfwd
ACN: Water (9:1)
DCM
DMF: Water (9:1)
DMF
ACN


DPE-II Solvent study cyclic voltammetry
0.000
-100.0
-200.0
-300.0
Current (µA)
-2.200 V
-1.800 V
-1.400 V
-1.000 V
-600.0 mV
-200.0 mV
Potential (V vs. Ref.)
ACN : Water (9:1)
DCM
ACN
DMF :Water (9:1)
DMF

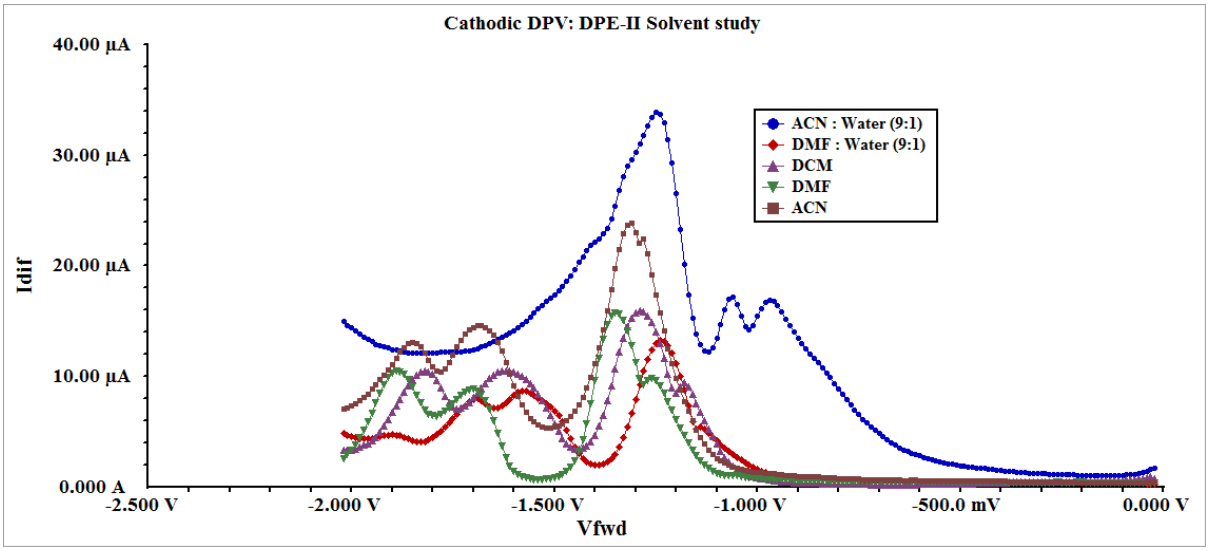


Figure S7 CV and DPV graphs of **DPE-I** and **DPE-II** with different solvent systems.