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Selective Electrochemical Detection of Bisphenol A using Molecular Imprinted Polymer Nanocomposite

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Table S1. Synthetic conditions used for making different nanocomposites.

Nanocomposite	Synthetic conditions	Bisphenol A detection sensitivity (µM)
MIPN	40 mg β-cyclodextrin acrylate, 3.8 mg bisphenol A, 50 mg AAm, 10 mg MBAA, 5 mg GO	0.02 to 20
NIPN	40 mg β-cyclodextrin acrylate, 50 mg AAm, 10 mg MBAA, 5 mg GO	0.5 to 20
MIPN1	20 mg β-cyclodextrin acrylate, 3.8 mg bisphenol A, 50 mg AAm, 10 mg MBAA, 5 mg GO	0.5 to 20
NIPN1	20 mg β-cyclodextrin, 50 mg AAm, 10 mg MBAA, 5 mg GO	0.5 to 20
MIPN2	40 mg β-cyclodextrin acrylate, 3.8 mg bisphenol A, 100 mg AAm, 5 mg MBAA, 5 mg GO	0.1 to 20
NIPN2	40 mg β-cyclodextrin, 100 mg AAm, 5 mg MBAA, 5 mg GO	0.5 to 20

Table S2. Comparison of molecular imprinting-based bisphenol A detection using this method and earlier reports.

Sensor materials	**Method**	**Linear range (µM)**	**LOD**	**Reference**
molecular imprinted TiO_2 single crystals	DPV	0.01-20	3.0 nM	19
molecular imprinted polymer-carbon nitride composite	CV	5-100	1.3 µM	30
molecularly imprinted polymer films	amperometric	0.0044-130	1.3 nM	31
molecularly imprinted nanobeads	potentiometric	0.5-13	0.15 µM	32
Molecularly imprinted polypyrrole-graphene	DPV	0.1-50	0.04 µM	33
magnetic particle-molecular imprinted polymer	impedance spectroscopy and CV	0.07-10	8.8 nM	35
molecular imprinted multi-walled carbon nanotube	DPV	4×10^{-3}-0.1 and 0.5-50	4.4 nM	36
molecularly imprinted chitosan–graphene	derivative voltammetry	0.008-1.0 and 1.0-20	6.0 nM	37
molecularly imprinted chitosan-acetylene black	DPV	0.005-0.20 and 0.50-10.00	2.0 nM	38
molecularly imprinted polymers-gold nanoparticle	CV and EIS	0.015-55	1.1 nM	39
molecular imprinted polymer nanocomposite	DPV	0.02-1.0	8 nM	This work

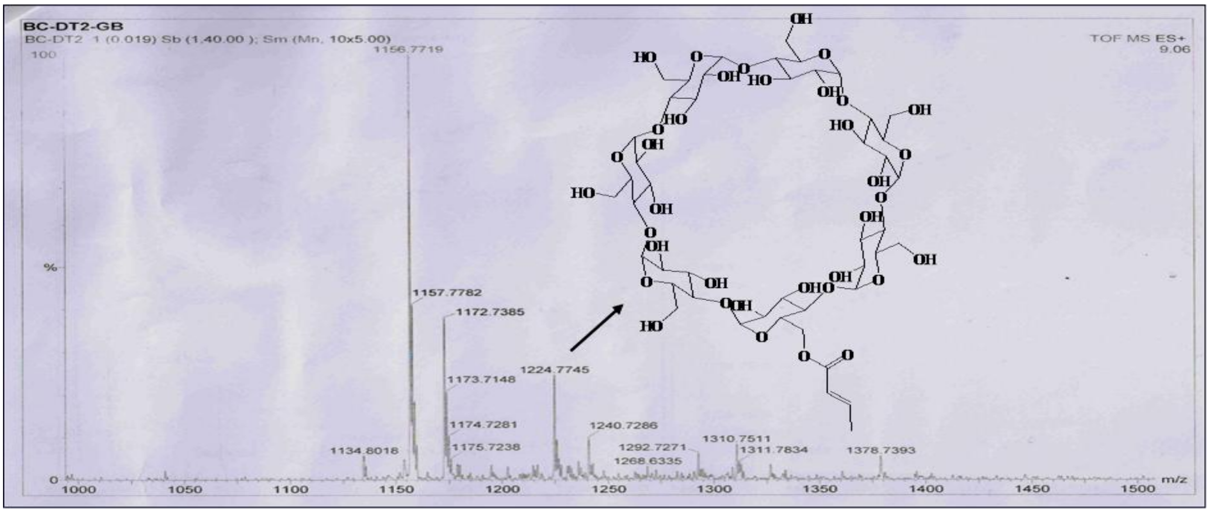

Figure S1. HRMS of β-cyclodextrin acrylate. The peak at 1224.7746 suggest the formation of β-cyclodextrin acrylate. [Calculated for $C_{46}H_{73}O_{36}Na$ ($M^+ + Na^+ - H^+$): 1224.71; found 1224.7746].

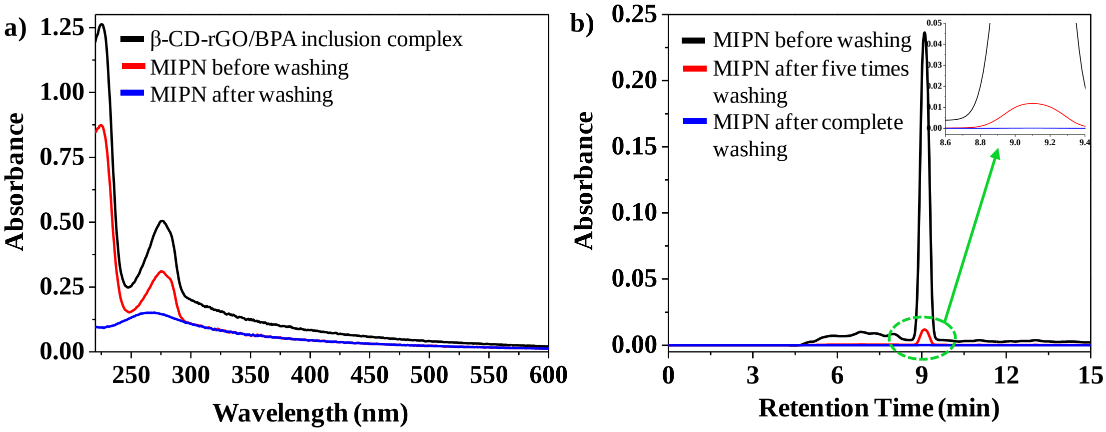

Figure S2. a) Absorbance spectra of MIPN in the different stages of synthesis, showing the complete removal of bisphenol A (BPA). b) HPLC data of BPA signal extracted from MIPN at different stages of washing. The peak at 9.0 min corresponds to BPA. (flow rate 0.5 mL/min, eluent is 90 % methanol-water and detection via UV absorption method). Inset shows the complete removal of BPA.

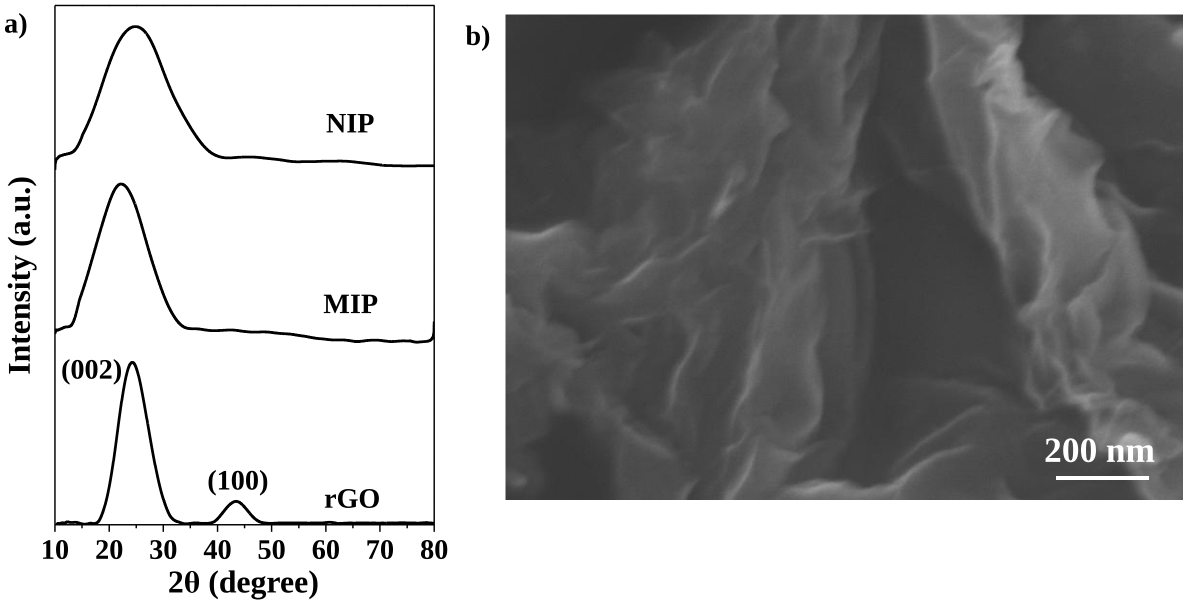

Figure S3. a) XRD patterns of rGO, MIPN and NIPN, showing the characteristic reflections at 2θ of 24° for (002) planes. The peak at 2θ of 24° indicates amorphous nature of the nanocomposites. b) FESEM image of reduced graphene oxide.

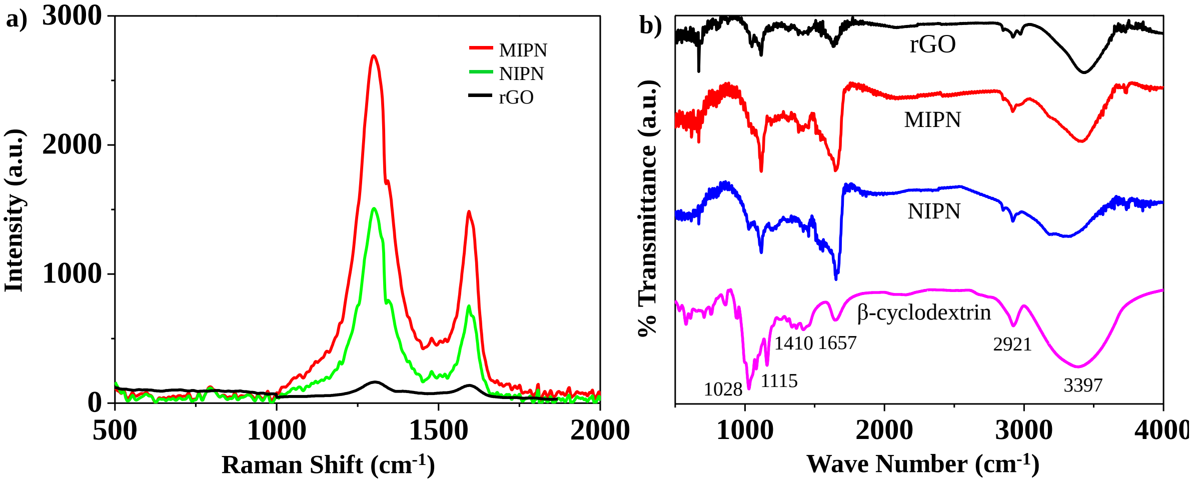

Figure S4. a) Raman spectra of MIPN/NIPN/rGO, showing the G band at ~ 1600 cm^{-1} that corresponds to sp^2 hybridized carbon atoms and D band at ~1300 cm^{-1} that corresponds to defective sp^2 hybridized carbon atoms. b) FTIR spectra of rGO, MIPN, NIPN and β-cyclodextrin, showing the presence of β-cyclodextrin in the nanocomposites.

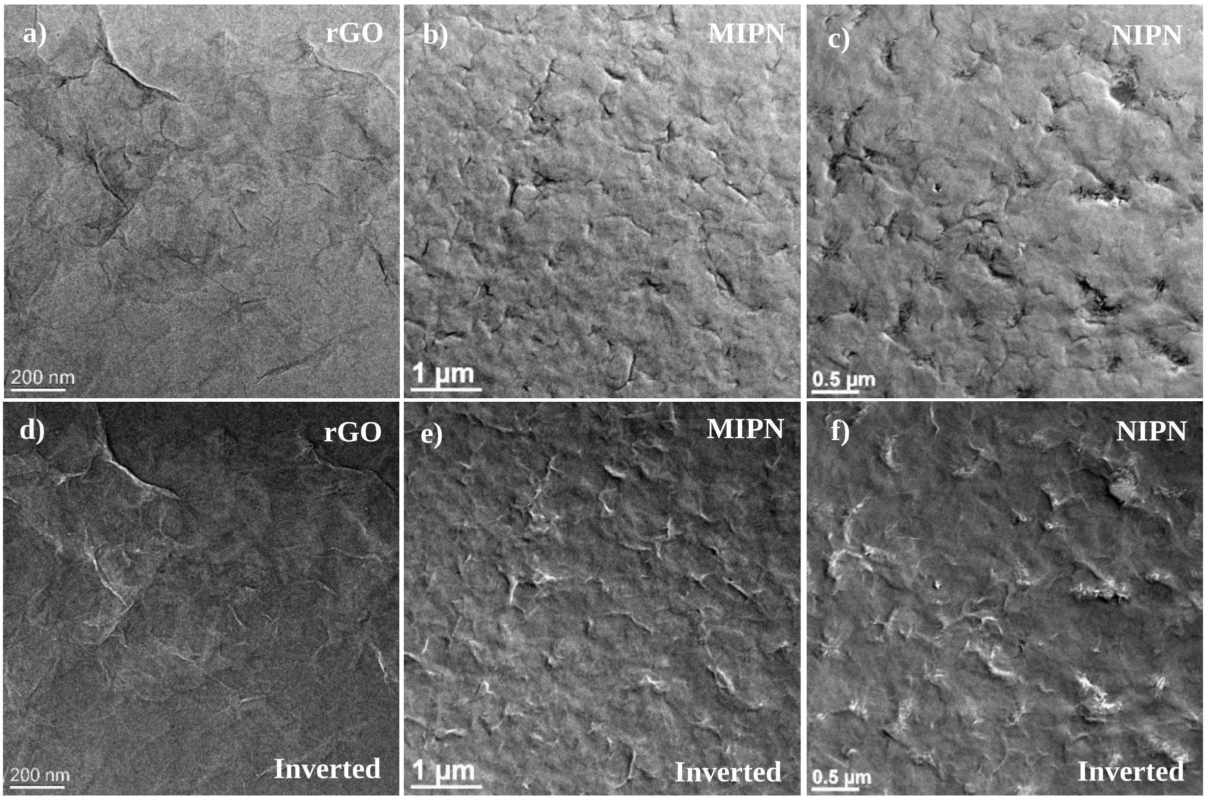

Figure S5. Low resolution TEM image (a-c) and corresponding inverted image (d-f) of rGO, MIPN and NIPN, showing the 3D structures of the MIPN/NIPN nanocomposites.

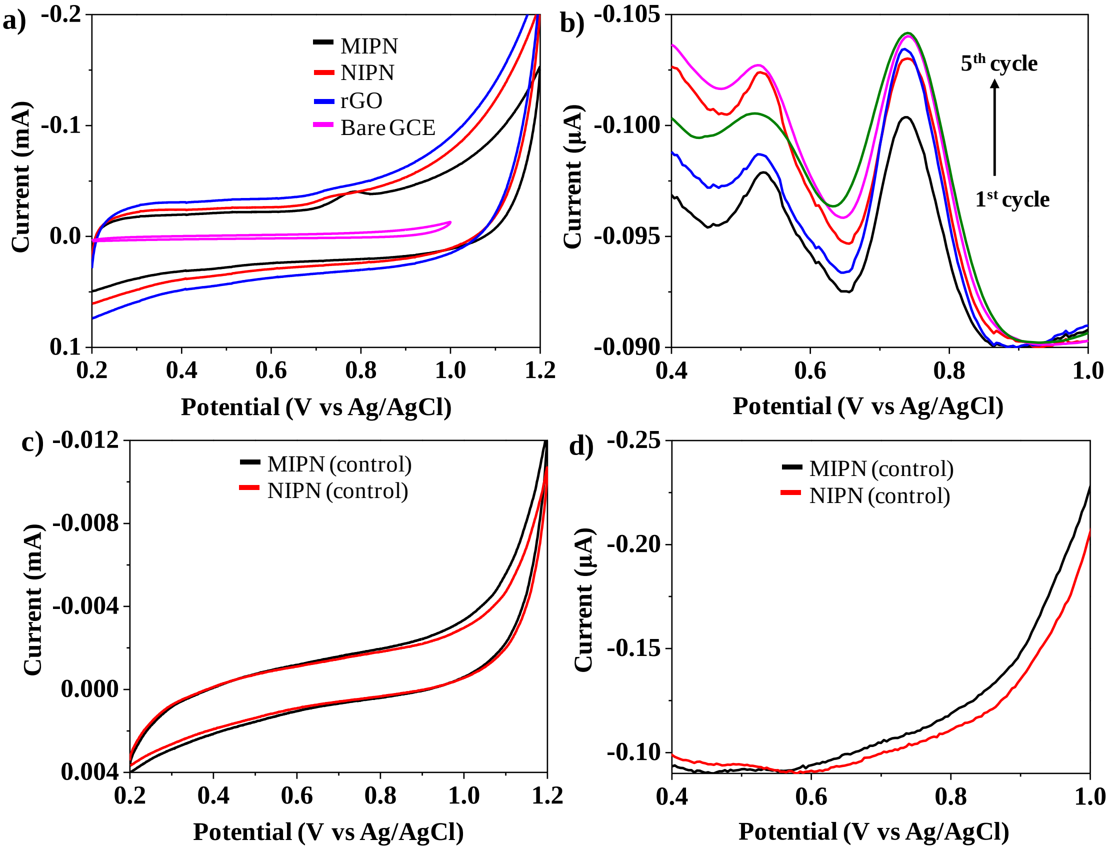

Figure S6. a) Cyclic voltammograms of different electrode in presence of 5 μM bisphenol A solution. b) Reproducible differential pulse voltammogram of BPA at different cycles using MIPN/GCE electrode, showing that MIPN/GCE can produce stable electrochemical signal of bisphenol A, even after five consecutive measurements. c) Cyclic voltammogram of control MIPN/NIPN prepared using cyclodextrin without acrylate modification in presence of 5 μM bisphenol A. d) DPV of 5 μM bisphenol A using control MIPN/NIPN.

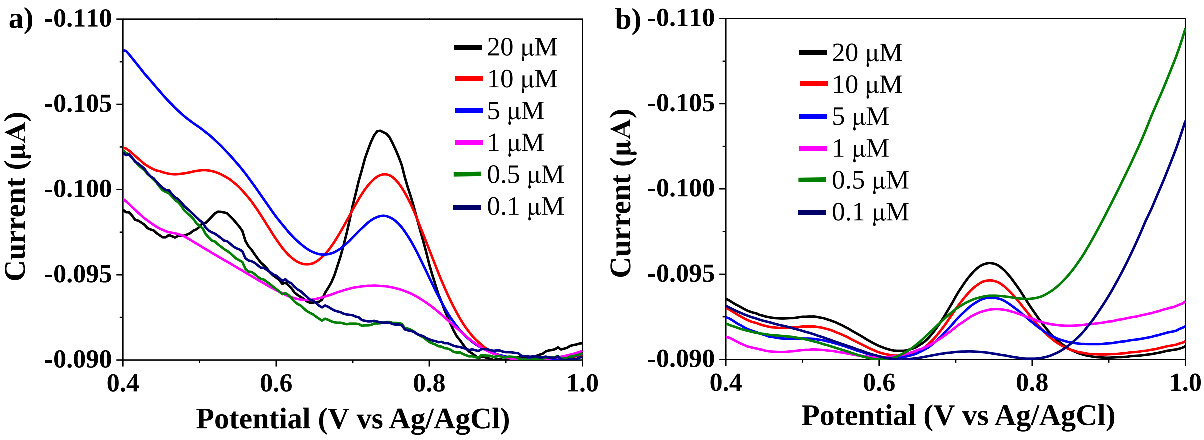

Figure S7. Differential pulse voltammograms at various concentration of bisphenol A in BR buffer 4.0 using GCE modified by MIPN1 (a) and NIPN1 (b). The peak at ~ + 0.74 V corresponds to bisphenol A oxidation peak.

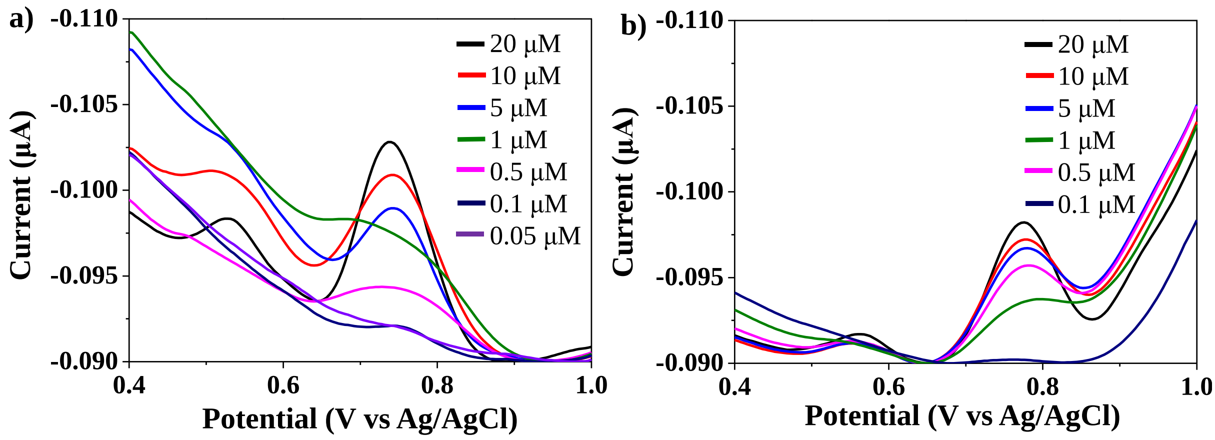

Figure S8. Differential pulse voltammograms at various concentration of bisphenol A in BR buffer 4.0 using GCE modified by MIPN2 (a) and NIPN2 (b).The peak at ~ +0.74 V corresponds to bisphenol A oxidation peak.

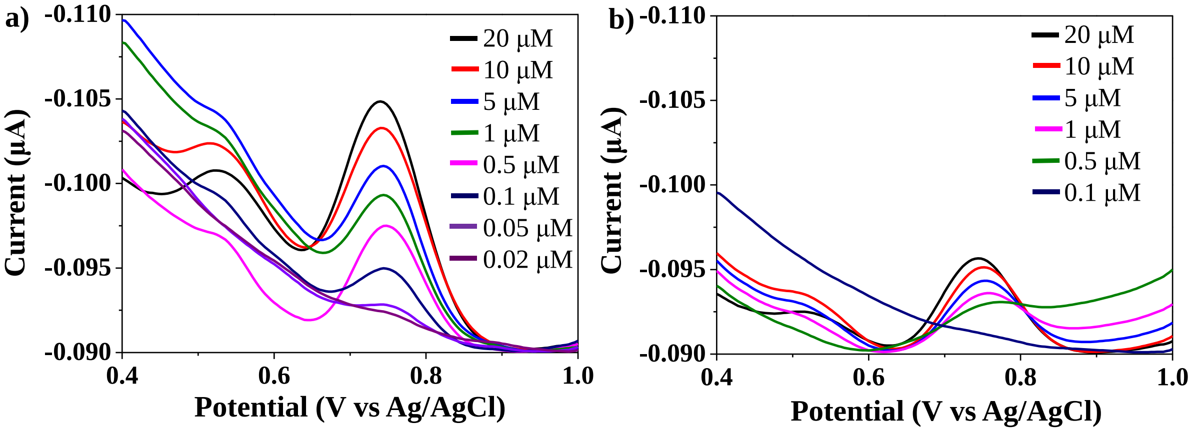

Figure S9. Differential pulse voltammograms at various concentration of bisphenol A in BR buffer 4.0 using GCE modified by MIPN (a) and NIPN (b) in presence of Tween 80 solution. The peak at ~ + 0.74 V corresponds to bisphenol A oxidation peak.

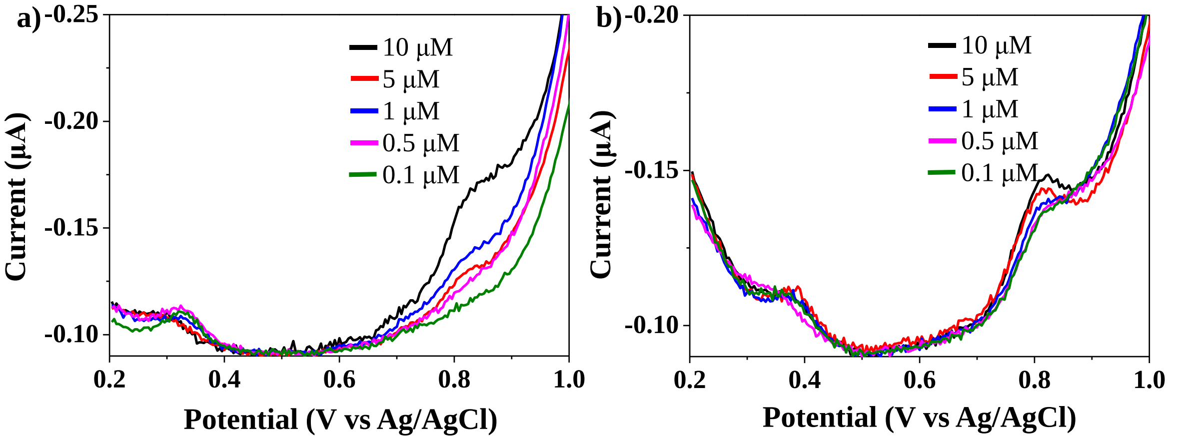

Figure S10. Differential pulse voltammograms at various concentration of BPAF using GCE modified by MIPN (a) and NIPN (b). The peak at ~ + 0.82 V corresponds to BPAF oxidation peak.

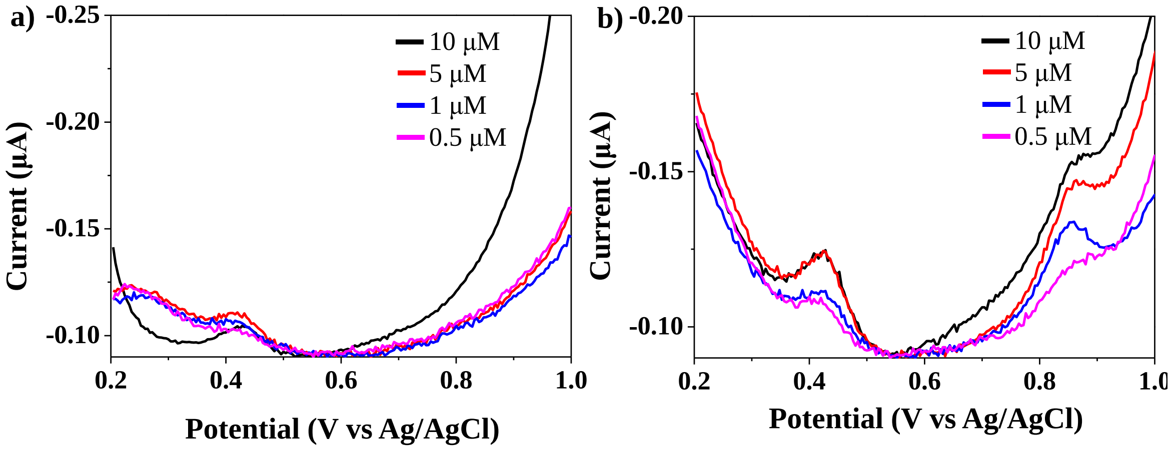

Figure S11. Differential pulse voltammograms at various concentration of BPB using GCE modified by MIPN (a) and NIPN (b). The peak at ~ + 0.85 V corresponds to BPB oxidation peak.

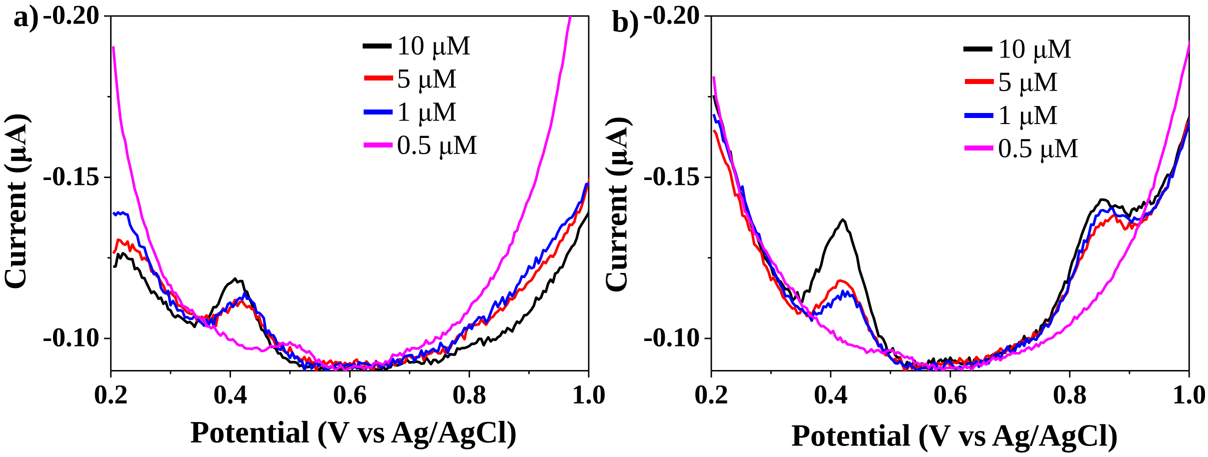

Figure S12. Differential pulse voltammograms at various concentration of DHBP using GCE modified by MIPN (a) and NIPN (b). The peak at ~ + 0.83 V corresponds to DHBP oxidation peak.

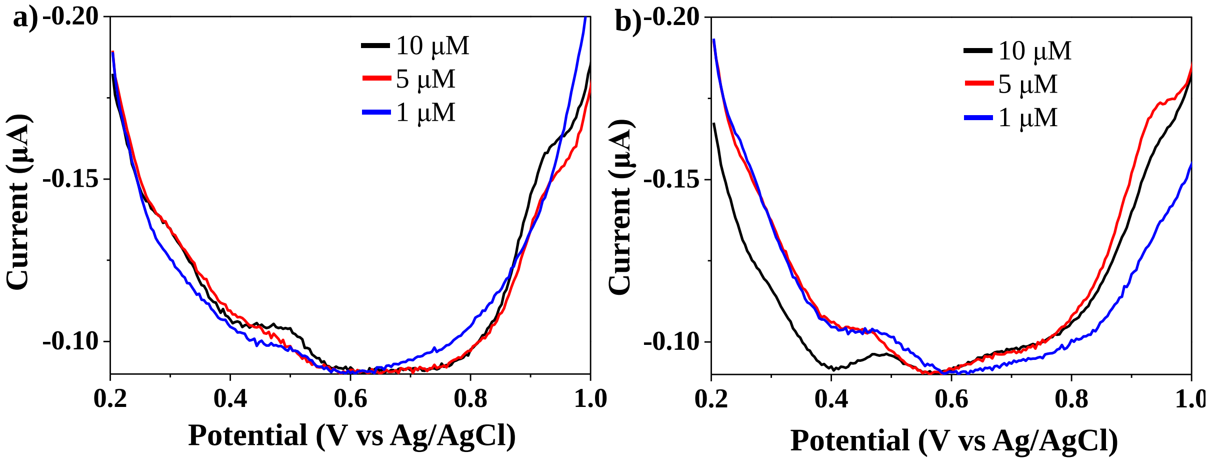

Figure S13. Differential pulse voltammograms at various concentration of phenol using GCE modified by MIPN (a) and NIPN (b). The band at ~ + 0.9 V corresponds to phenol oxidation peak.

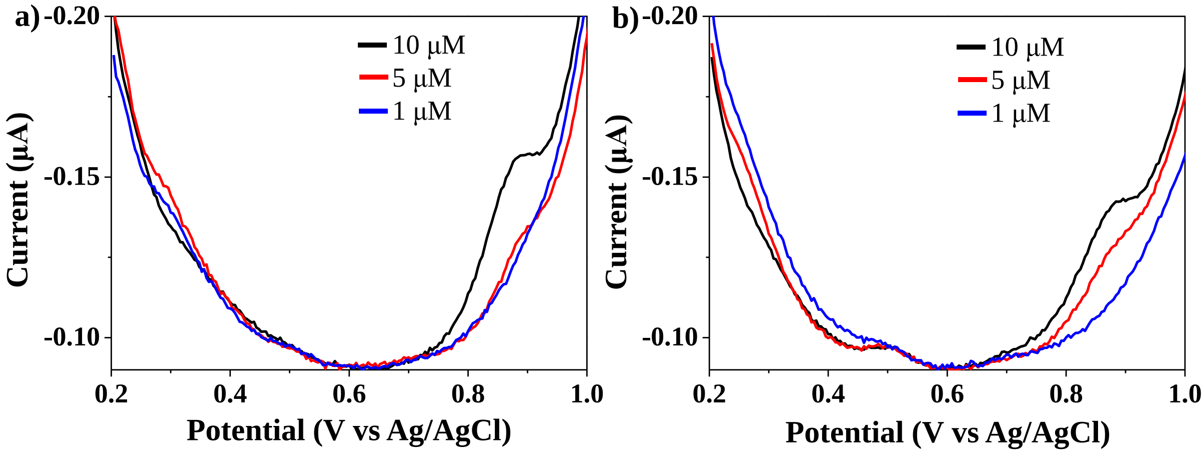

Figure S14. Differential pulse voltammograms at various concentration of resorcinol in BR buffer 4.0 using GCE modified by MIPN (a) and NIPN (b). The peak at ~ + 0.9 V corresponds to resorcinol oxidation peak.

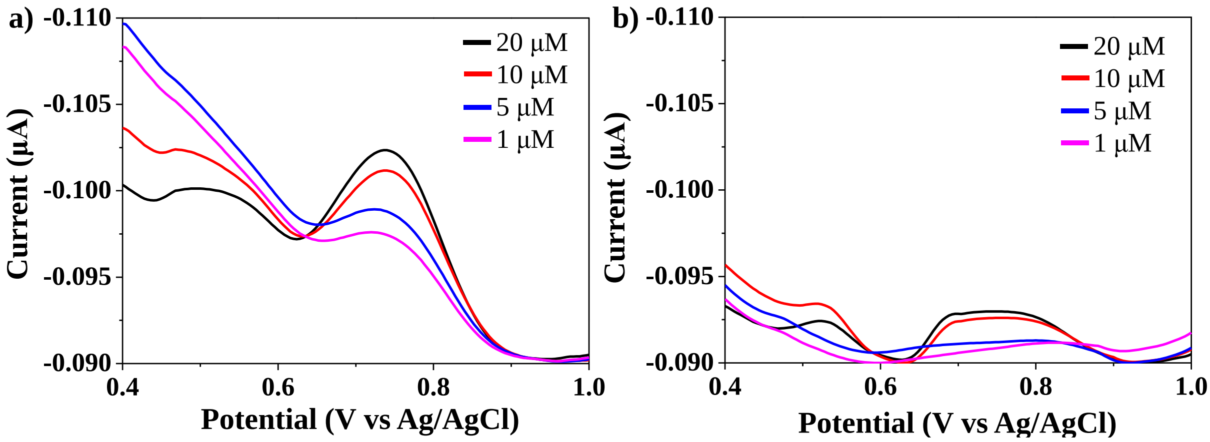

Figure S15. Differential pulse voltammograms at various concentration of bisphenol A using GCE modified by MIPN (a) and NIPN (b) in presence of 5 μM BPAF solution.

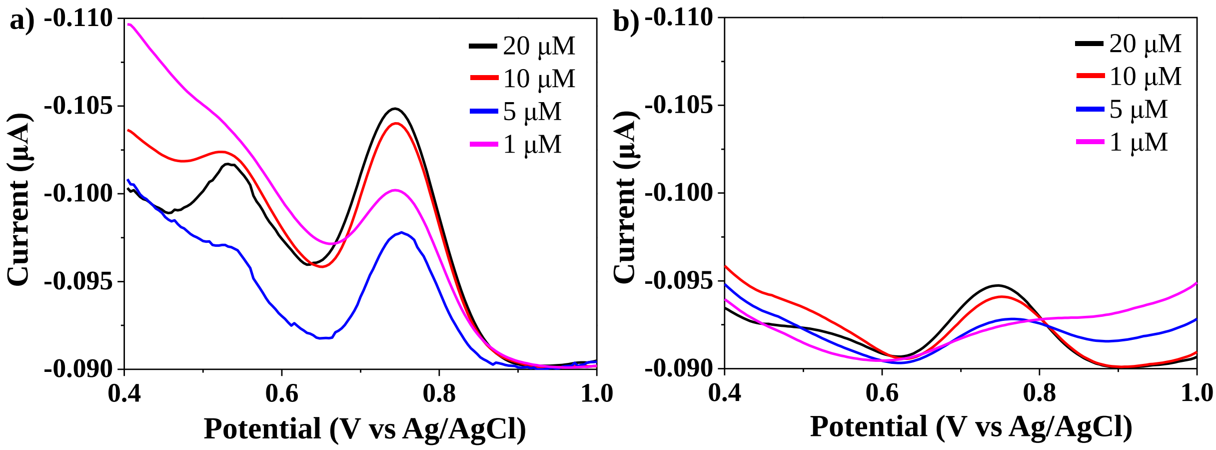

Figure S16. Differential pulse voltammograms at various concentration of bisphenol A using GCE modified by MIPN (a) and NIPN (b) in presence of 5 μM BPB solution.

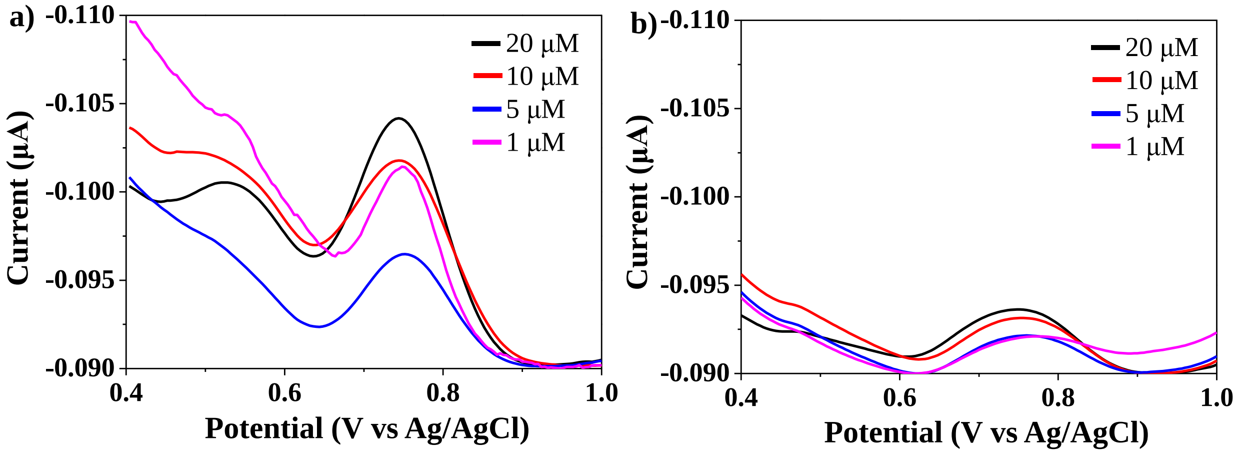

Figure S17. Differential pulse voltammograms at various concentration of bisphenol A using GCE modified by MIPN (a) and NIPN (b) in presence of 5 μM DHBP solution.

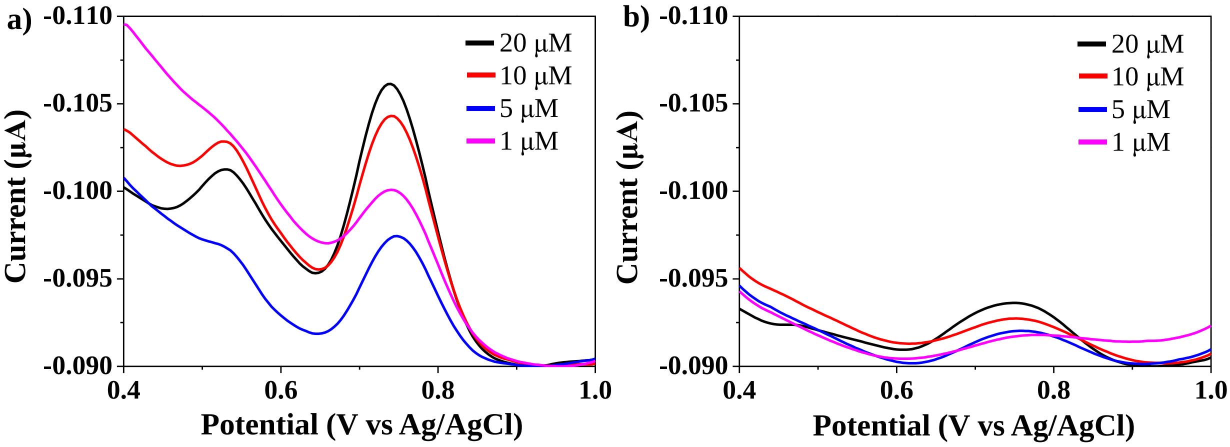

Figure S18. Differential pulse voltammograms at various concentration of bisphenol A using GCE modified by MIPN (a) and NIPN (b) in presence of 5 µM phenol solution.

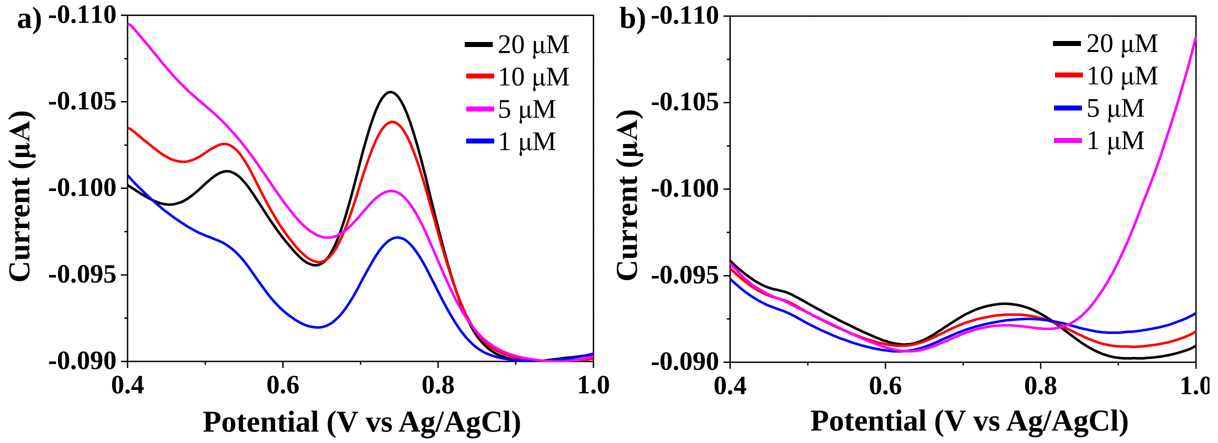

Figure S19. Differential pulse voltammograms at various concentration of bisphenol A using GCE modified by MIPN (a) and NIPN (b) in presence of 5 µM resorcinol solution.