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ELECTRONIC SUPPORTING INFORMATION

Homopolymerization of 3-aminobenzoic acid for enzymeless electrocatalytic assay of nitrite

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S1: Electropolymerization Optimization

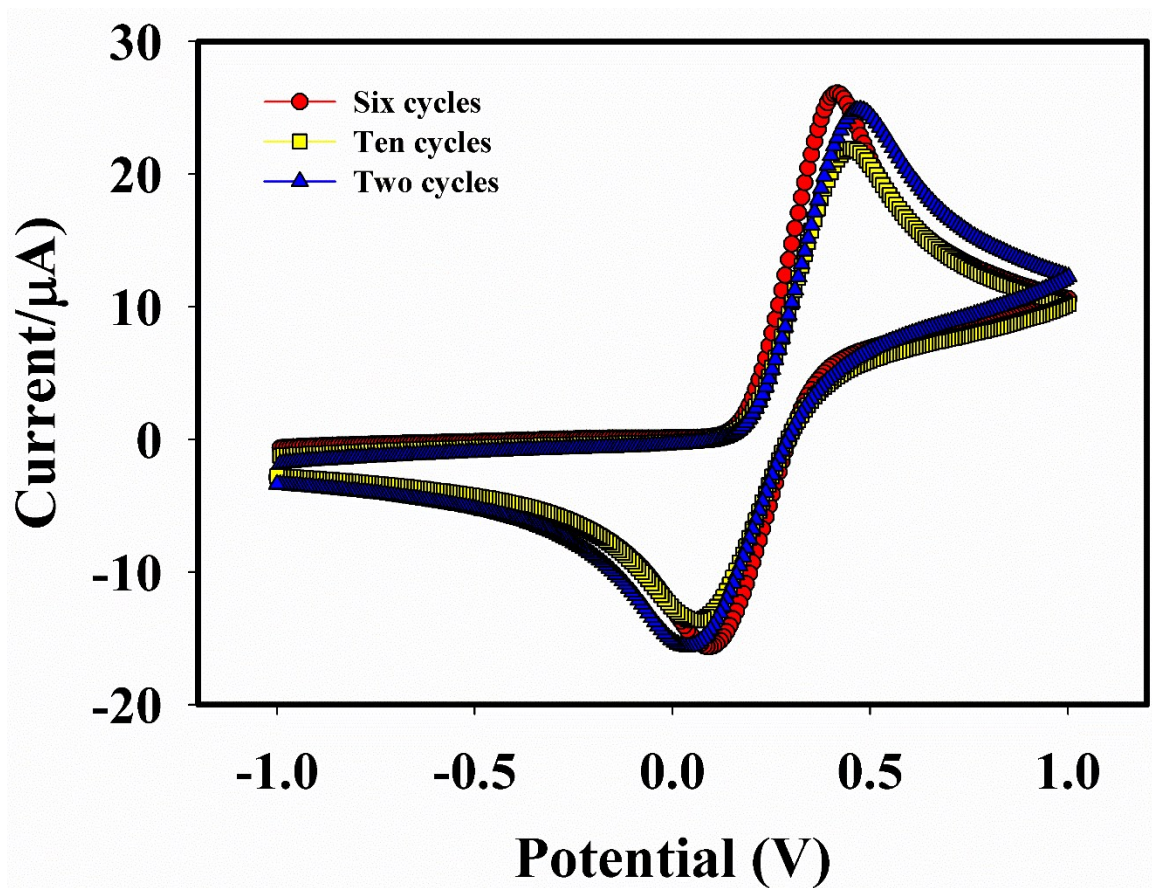


Fig.S1: cyclic voltametric behaviour of poly (3-aminobenzoic acid) synthesized at different number of voltammetric cycles or sweep in $0.1\text{mM Fe (CN)}_6^{3-/4-}$

Table S1: The oxidation current of PABA synthesized by varying number of cyclic voltammetric sweep.

No of cycles	Oxidation peak current (μA)	Oxidation potential (V)
2	21.9073	0.4501
6	26.0771	0.4172
10	24.8391	0.4749

S2: Results of XPS analysis

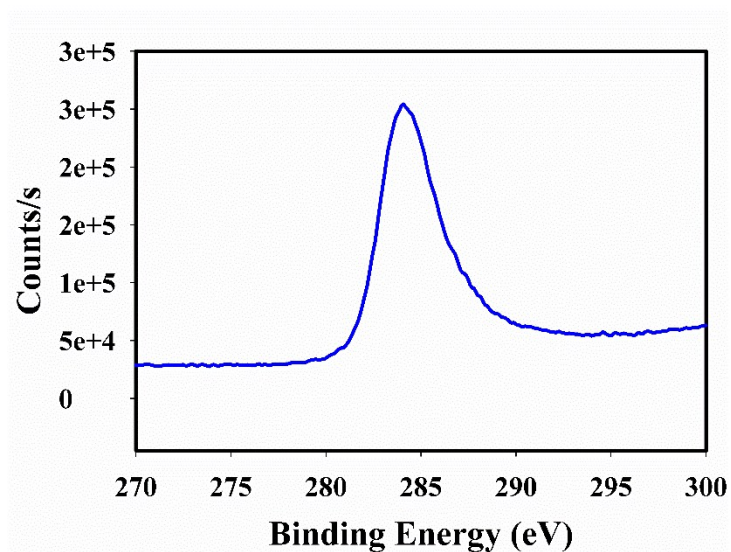


Fig.S2a. XPS spectra for C1s.

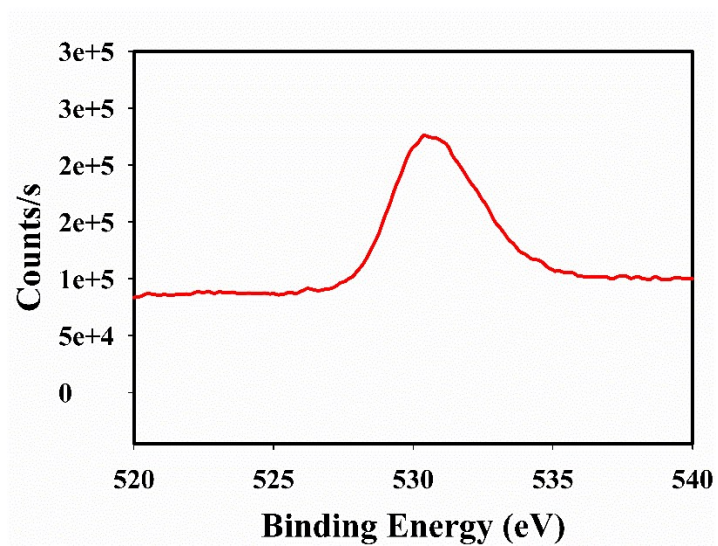


Fig.S2b. XPS spectra for O1s

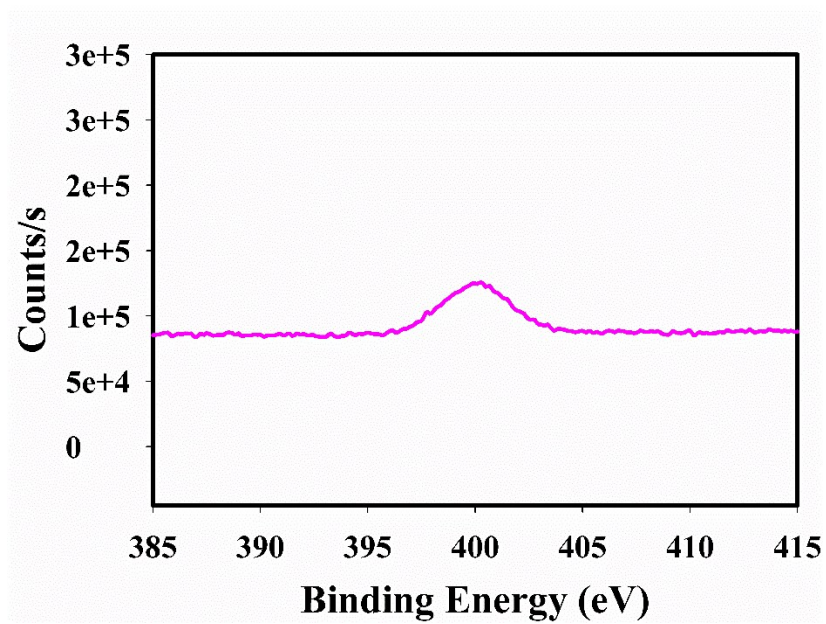


Fig.S2c.XPS spectrum showing N1s

S3: Supporting electrolyte (PBS) variation and optimization

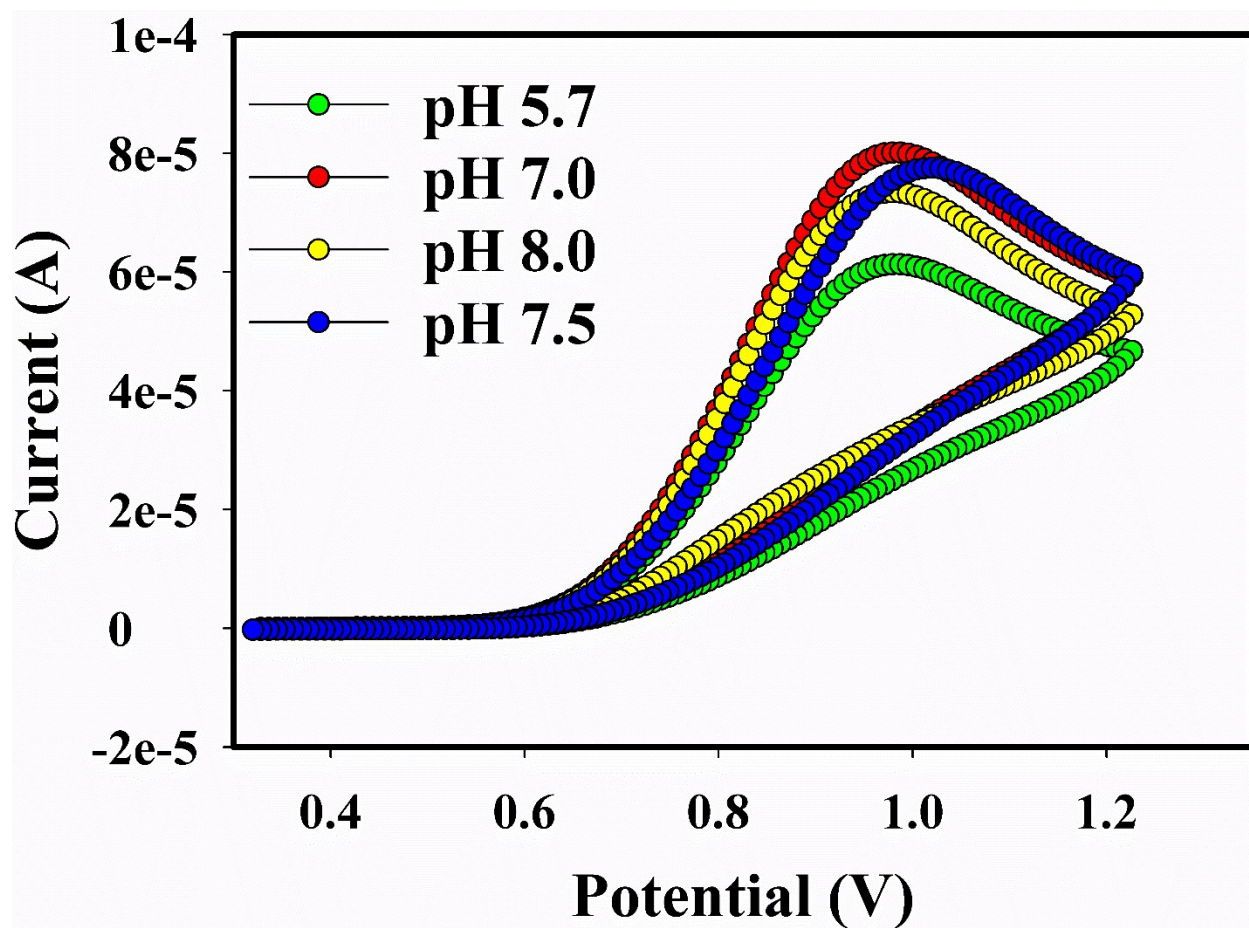


Fig. S3: Effect of pH variation on oxidation current response of PABA in 0.25mM NO_2^-

S4: Analytical performance parameters

Limit of Detection (LOD)

This was calculated using the equation;

$$\text{LOD} = \frac{3 \times \text{SD}}{\text{Slope of the calibration plot}}$$

where SD is the standard deviation of the blank response.

From our results, $\text{LOD} = 3 \times 1.53 \times 10^{-8} / 0.3 = 0.15 \mu\text{M}$

Limit of Quantification (LOQ)

This was determined using the equation.

$$\text{LOQ} = \frac{10 \times \text{SD}}{\text{Slope of the calibration plot}}$$

$\text{LOQ} = 10 \times 1.53 \times 10^{-8} / 0.3 = 0.51 \mu\text{M}$

Sensitivity

This was calculated using the formula:

$$\text{Sensitivity} = \frac{\text{Slope of the calibration plot}}{\text{GCE surface area}}$$

$\text{Sensitivity} = 0.3 \mu\text{A} \mu\text{M}^{-1} / 0.2 \text{cm}^2 = 1.53 \mu\text{A} \mu\text{M}^{-1} \text{cm}^{-2}$

Linear dynamic range (LDR)

The calibration plot was linear till addition of 140 μ M

Full dynamic range (FDR)

The full calibration range was 10-140 μ M

S4-1: Kinetic studies of detection of nitrite on poly(3-ABA) modified GCE

Tafel slope:

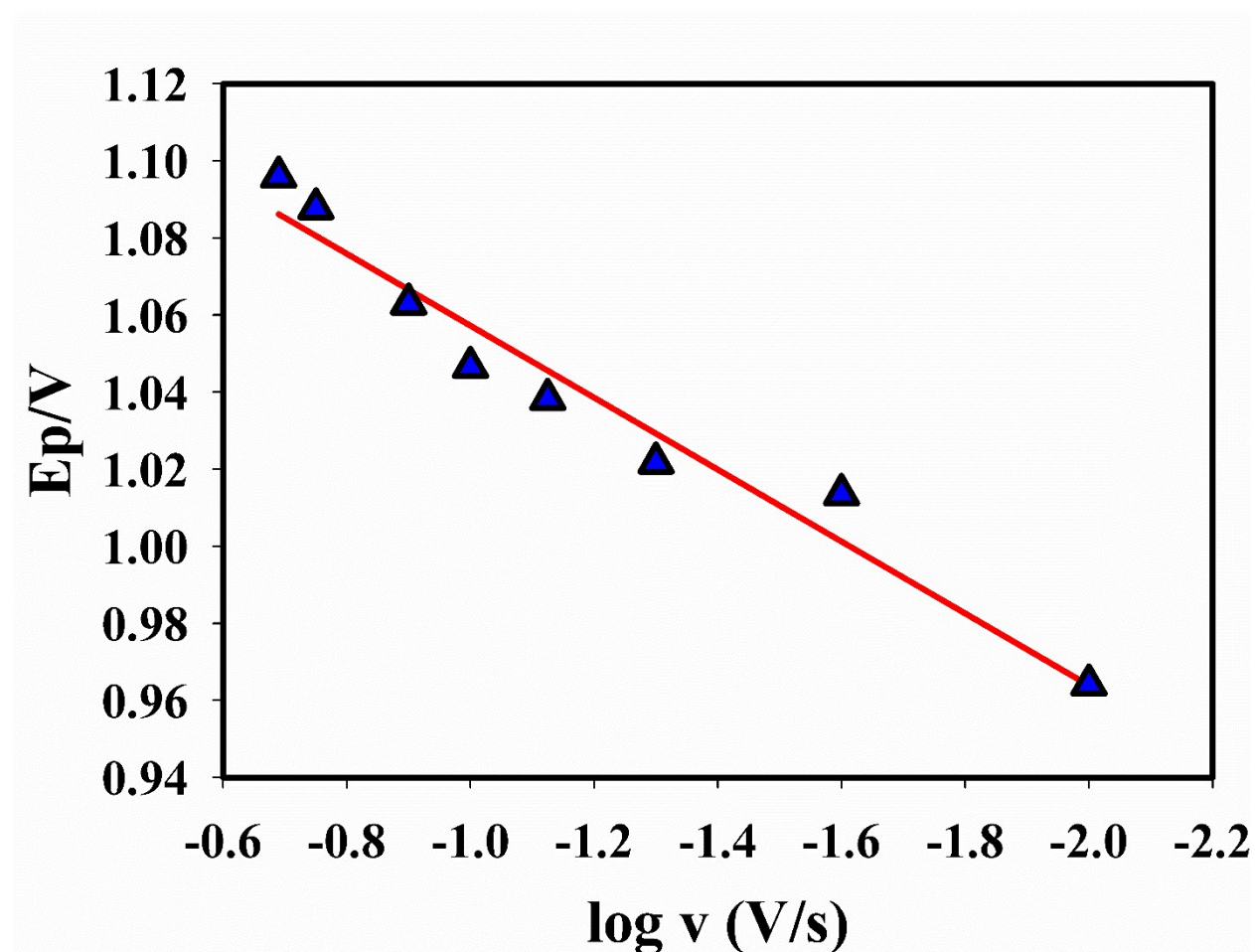


Figure S4a: Plot of peak potential against logarithm of the scan rate.

The equation of the plot:

$$E_p \text{ (V)} = 0.03 \times \log v \text{ (V/s)} + 1.16$$

$$E_p = \frac{b(\log v)}{2} + C.$$

Using the slope of the plot and the equation given above, Tafel slope is calculated as:

$$b = 60 \text{ mV/dec.}$$

Charge transfer coefficient (α)

$$\alpha = \frac{47.7}{(E_p - \frac{E_p}{2})} \text{ mV}$$

$$= 47.7 / (950 - 850) \text{ mV}$$

$$= 47.7 / 100 = 0.47$$

Diffusion coefficient (D)

D was calculated using Randles sevcik equation

$$i_p = 2.69 \times 10^5 \text{ A n}^{3/2} \text{ C D}^{1/2} v^{1/2}$$

$$D = 4.65 \times 10^{-8} \text{ cm}^2/\text{s}$$

S4-2: Stability Assessment

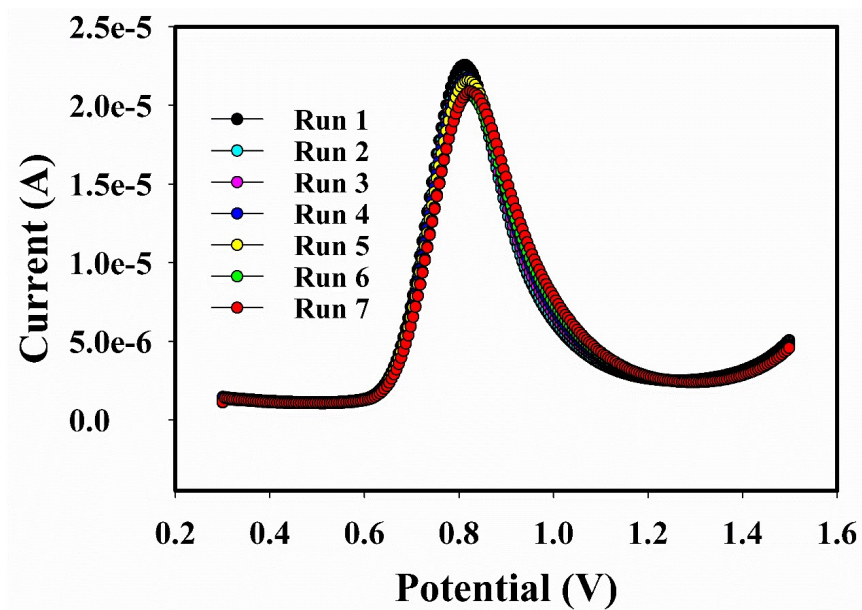


Fig. S4b: The current response of PABA in 60 μM NO_2^- for seven consecutive readings

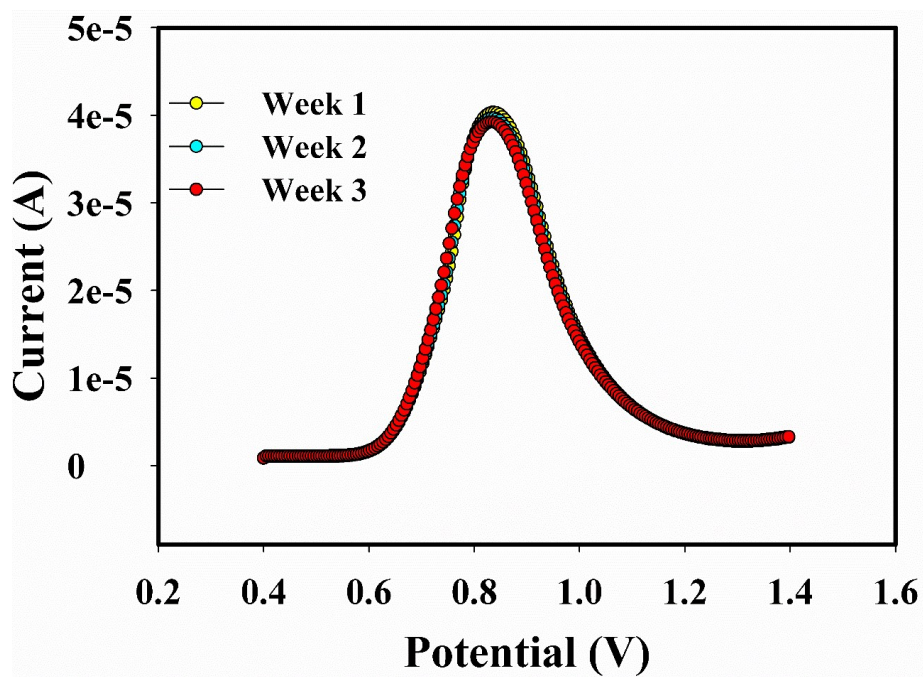


Fig. S4c: The current response of PABA in 120 μM NO_2^- for three consecutive weeks

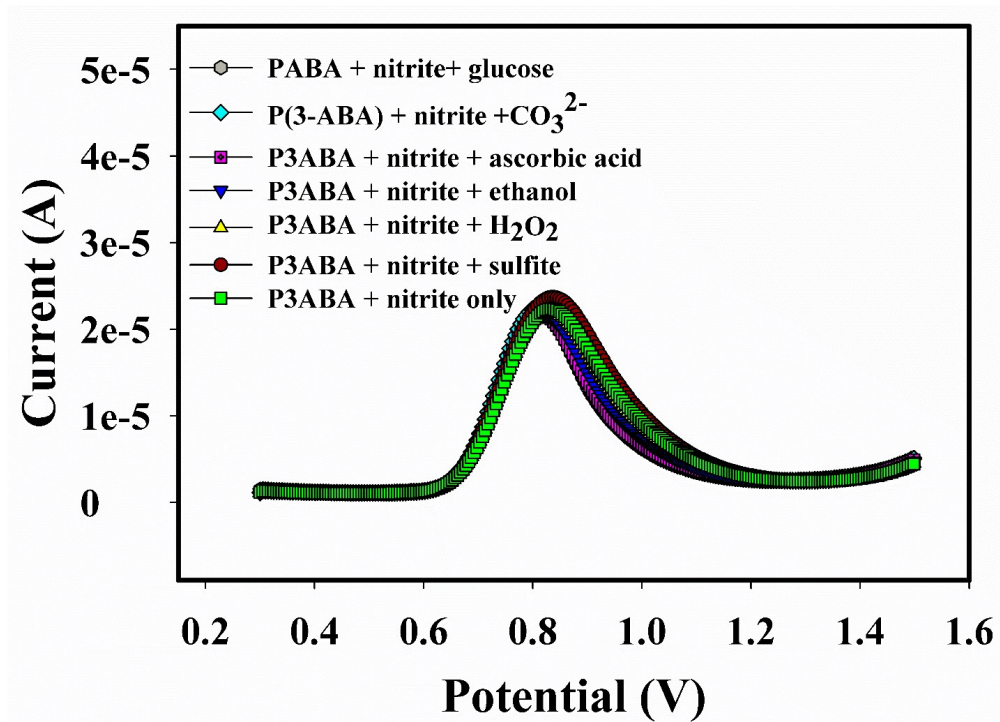


Fig.S4d. Current response of poly(3-ABA) in 60μM nitrite in the absence and presence of likely interferents (same fold concentration)

S5: Statistical Analysis

Repeatability measurements

The oxidation peak currents: 2.2568e-5, 2.1857e-5, 2.1738e-5, 2.1747e-5, 2.1588e-5, 2.0660e-5 and 2.0898e-5.

Mean value = 2.153e-5

$$\text{Standard deviation, } \sigma = \sqrt{\frac{\sum (X - \bar{X})^2}{n - 1}}$$

Sd = 6.142e-7

$$\text{Relative standard deviation (RSD)\%} = \frac{Sd}{X (\text{mean value})} \times 100$$

$$= \frac{6.142 \times 10^{-7}}{2.15 \times 10^{-5}} \times 100$$

$$= 2.86\%$$

Reproducibility measurement

The oxidation peak currents obtained are:

4.0314e-5; 3.9246e-5 and 3.9703e-5

Mean = 3.98e-5

$$\text{RSD \%} = \frac{4.38 \times 10^{-7}}{3.98 \times 10^{-5}} \times 100$$

$$= 1.01\%$$

Interference

The oxidation peak currents recorded were:

2.186e-5 (nitrite only), 2.368e-5, 2.173e-5, 2.188e-5, 2.186e-5, 2.168e-5, 2.170e-5

Mean value = 2.201e-5

Sd = 1.36×10^{-6}

$$\text{RSD \%} = \frac{1.36 \times 10^{-6}}{2.201 \times 10^{-5}} \times 100$$

$$= 2.95\%$$

S6: Real sample analysis

Method used: Standard addition.

$$Recovery (\%) = \frac{C_i - C_o}{C_s}$$

Where C_i is the total concentration of analyte, C_o is concentration of analyte (before spike), C_s is the concentration of the spiked nitrite