

Supplementary Material

Smartphone-Controlled Aptasensor for Voltammetric Detection of Patulin in Apple Juice

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Safety information

Patulin: GSH06; Hazard Classifications: Acute Tox. 2 Oral - Skin Irrit. 2; Hazard Statements: H300 - H315; Storage Class Code: 6.1A - Combustible, acute toxic Cat. 1 and 2 / very toxic hazardous materials; WGK: WGK3

Fumonisin B1: GHS02,GHS07; Hazard Classifications: Acute Tox. 4 Oral - Eye Irrit. 2 - Flam. Liq. 2; Hazard Statements: H225 - H302 - H319; Storage Class Code: 3 - Flammable liquids; WGK: WGK 2

Deoxynivalenol: GHS02,GHS07; Hazard Classifications: Acute Tox. 4 Dermal - Acute Tox. 4 Inhalation - Acute Tox. 4 Oral - Eye Irrit. 2 - Flam. Liq. 2; Hazard Statements: H225 - H302 + H312 + H332 - H319; Storage Class Code: 3 - Flammable liquids; WGK: WGK 2

Ochratoxin A: GHS02,GHS07; Hazard Classifications: Acute Tox. 4 Dermal - Acute Tox. 4 Inhalation - Acute Tox. 4 Oral - Eye Irrit. 2 - Flam. Liq. 2; Hazard Statements: H225 - H302 + H312 + H332 - H319; Storage Class Code: 3 - Flammable liquids; WGK: WGK 2

Table S1. The average current values ($n=3$) of redox probe with % RSD and the change ratio (%) at current value obtained before/after aptamer immobilization onto the electrode (PGE) surface at different concentrations of DNA aptamer.

	I (μA) and RSD (%)	Change ratio (%) at current
PGE (Control group)	212.59 \pm 2.75 1.29 %	
0.25 μ g/mL Aptamer/PGE	203.52 \pm 0.60 0.29 %	4.27 Decrease
1 μ g/mL Aptamer/PGE	194.76 \pm 17.29 8.88 %	8.39 Decrease
2.5 μ g/mL Aptamer/PGE	141.11 \pm 6.30 4.46 %	33.62 Decrease
5 μ g/mL Aptamer/PGE	149.55 \pm 13.72 9.17 %	29.65 Decrease

Table S2. The average current values ($n=3$) of redox probe with % RSD and the change ratio (%) at current value obtained before/after aptamer immobilization onto the electrode surface in different immobilization times and after interaction of aptamer with PAT.

	I_{APT} (μA) and RSD (%)	I_{APT-PAT} (μA) and RSD (%)	Change ratio (%) at current
30 min	142.07 ± 2.10	149.41 ± 13.86	5.17 Increase
immobilization	1.48 %	9.28 %	
60 min	141.11 ± 6.30	99.62 ± 13.41	29.41 Decrease
immobilization	4.46 %	13.46 %	

Table S3. The average current values ($n=3$) of redox probe with % RSD and the change ratio (%) at current value obtained before/after aptamer interaction with PAT in different interaction times.

	I_{APT} (μA) and RSD (%)	I_{APT-PAT} (μA) and RSD (%)	Change ratio (%) at current
15 min interaction		106.84 ± 21.63	24.29 Decrease
		20.25 %	
30 min interaction	141.11 ± 6.30	99.62 ± 13.41	29.41 Decrease
	4.46 %	13.46 %	
60 min interaction		102.73 ± 9.30	27.20 Decrease
		9.05 %	

Limit of detection

In this study, the limit of determination was calculated according to the IUPAC method [1].

The analyte's signal at the detection limit (Sdl) is given by:

$$Sdl = S_{reag} + k * \sigma_{reag},$$

where S_{reag} is the electrochemical signal for a blank, σ_{reag} is the known standard deviation for the blank's electrochemical signal ($n_{\sigma}=3$ for buffer medium and $n_{\sigma}=3$ for apple juice medium).

k is a numerical factor chosen according to the confidence level desired. In this study k value was selected as $k=3$ (99.86 % confidence level) according to the Long and Winefordner [2].

In our study, S_{reag} is the electrochemical signal for a blank (aptamer control), σ_{reag} is the known standard deviation for the electrochemical signal of aptamer control ($n_{\sigma}=3$ for buffer medium and $n_{\sigma}=3$ for apple juice medium). The electrochemical signal of redox probe (current; I , μA) used to calculate LOD were presented in Table S4 and Table S5 for buffer medium and apple juice medium, respectively. The detection limit of aptasensor was achieved as 0.18 pg/mL in buffer medium and 0.47 pg/mL in apple juice medium by the data given in Table S4 and Table S5, formula and calibration curves.

Table S4. The electrochemical signal of redox probe presenting the values (I , μA) of the blank for three times in buffer medium.

Number	I (μA)	Average (μA)	SD (μA)	RSD (%)
1	121.18	120.31	0.88	0.73
2	120.32			
3	119.42			

Table S5. The electrochemical signal of redox probe presenting the values (I , μA) of the blank for three times in apple juice medium.

Number	I (μA)	Average (μA)	SD (μA)	RSD (%)
1	146.54	146.96	0.37	0.25
2	147.18			
3	147.17			

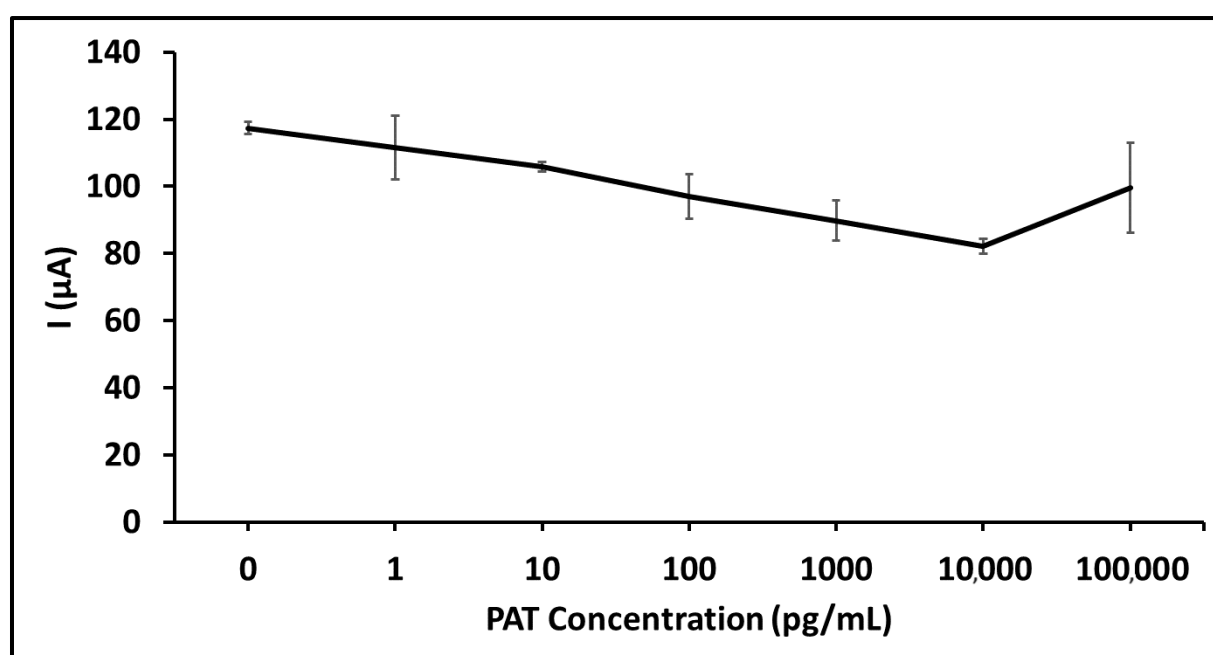


Figure S1. Line graph representing the average current values ($n=3$) of redox probe obtained with increasing concentration of PAT in buffer medium (50 mM PBS, pH 7.4).

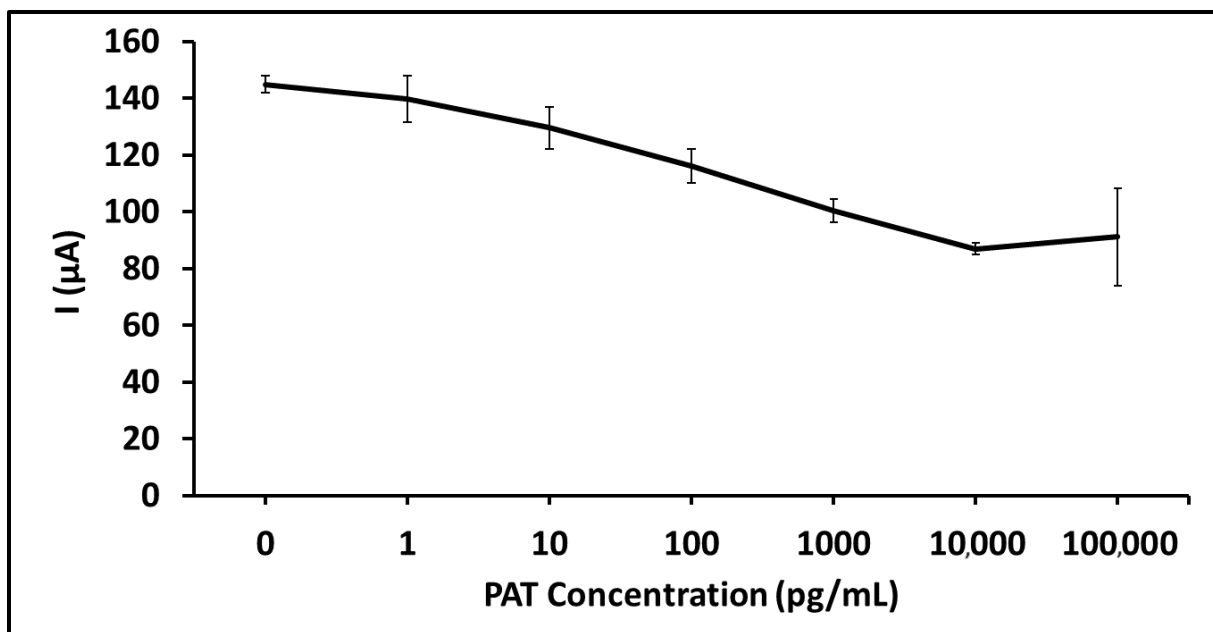


Figure S2. Line graph presenting the average current values ($n=3$) of redox probe measured by smartphone connected to portable device while increasing the concentration of PAT (1 to 10^5 pg/mL) prepared in diluted apple juice medium.

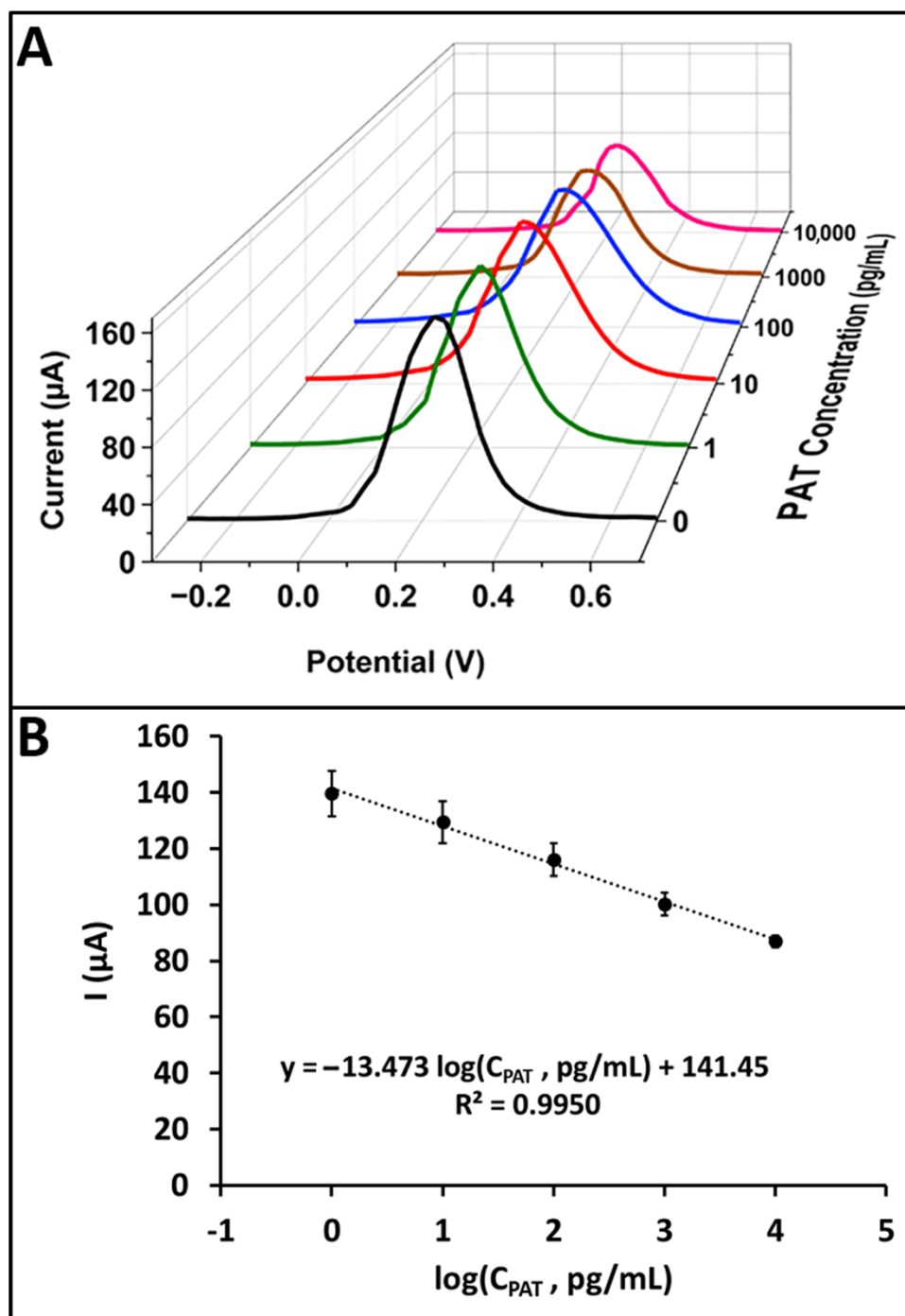


Figure S3. (A) Representative voltammograms of redox probe signal recorded by using a smartphone integrated to portable device in the concentration range of PAT varying from 1 pg/mL to 10^4 pg/mL prepared in diluted apple juice medium (1:50). The voltammograms in black, green, red, blue, brown and pink colour represent 0 pg/mL (blank), 1 pg/mL , 10^1 pg/mL ,

10^2 pg/mL, 10^3 pg/mL and 10^4 pg/mL PAT, respectively. (B) Calibration plot based on the data for detection of PAT in apple juice medium by using smartphone integrated to portable device.

Table S6. Reproducibility of PAT aptasensor using a smartphone integrated to portable device in apple juice medium in three different days.

10,000 pg/mL PAT	I (μ A)	RSD (% , $n=6$)
1st day	85.81	5.23
	84.61	
2nd day	78.25	
	89.44	
3rd day	78.79	
	85.67	

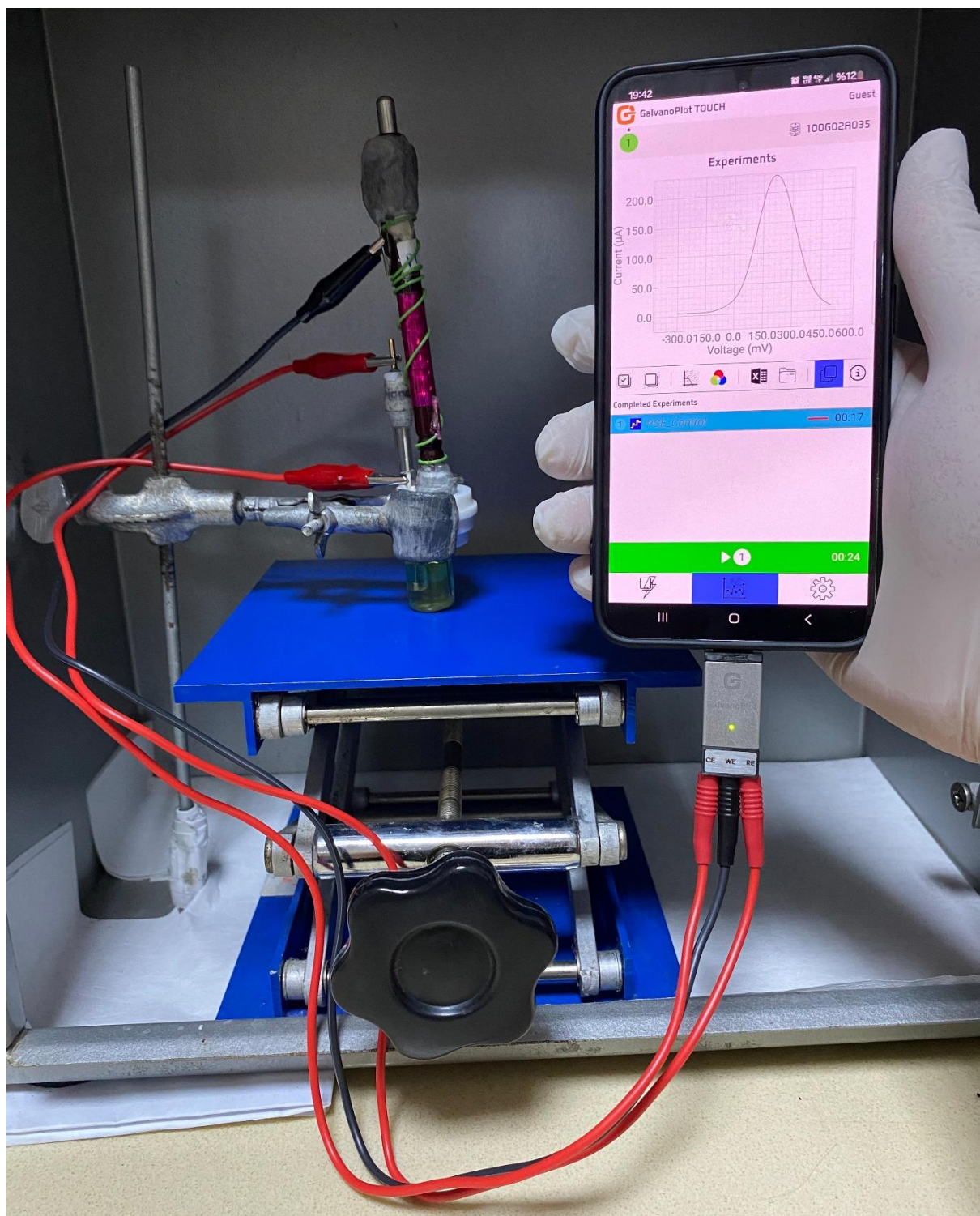


Figure S4. Picture of the set-up of the smartphone integrated portable device.

References

1. IUPAC Nomenclature, Symbols, Units and Their Usage in Spectrochemical Analysis—
Iii. Analytical Flame Spectroscopy and Associated Non-Flame Procedures. *Pure Appl. Chem.* **1976**, *45*, 105–123, doi:10.1351/pac197645020105.
2. Long, G.L.; Winefordner, J.D. Limit of Detection A Closer Look at the IUPAC Definition. *Anal. Chem.* **1983**, *55*, 712–714.