

SUPPLEMENTARY MATERIAL

MoS₂/PPy nanocomposite as transducer for electrochemical aptasensor of ampicillin in river water

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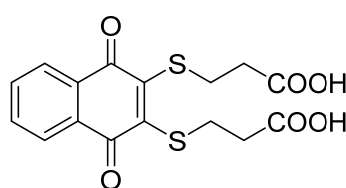
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SI.1. Material and methods

SI.1.1. Synthesis of the naphthoquinone derivative



¹H NMR (d6-DMSO) δ 2.65–2.69 (t, 2H), 3.11–3.12 (t, 2H), 6.77 (s, 1H), 7.81–7.86 (m, 2H), 7.95–7.97 (m, 2H); ¹³C NMR (d6-DMSO) δ 24.76, 31.95, 126.03, 126.34, 127.28, 131.43, 131.68, 133.65, 134.74, 153.40, 172.48, 180.95, 181.83;

SI.1.2. Preparation of MoS₂ nanosheets

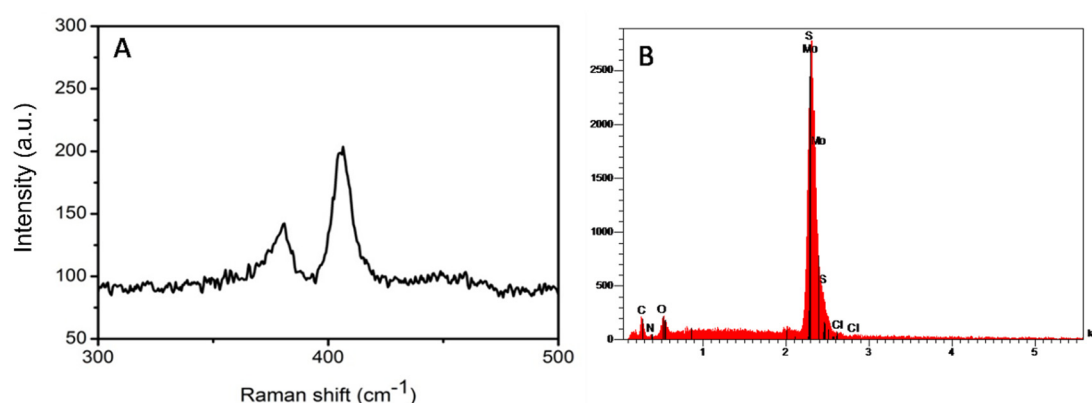


Figure S1. (A) Raman Spectra of MoS₂ nanosheets and (B) EDX analysis of the modified SPCE with MoS₂ nanosheets

SL.1.3. Electrodeposition of MoS₂ on SPCE

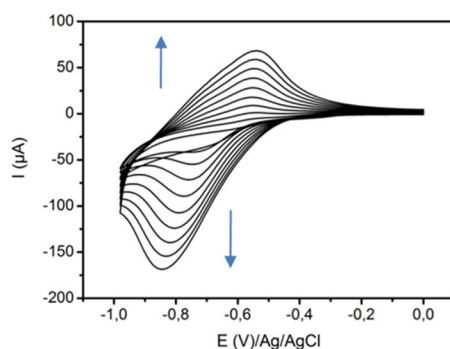


Figure S2. Electrodeposition of MoS₂ by cycling the potential between -0.1V and -0.95V, for 10 cycles at scan rate 100 mV.s⁻¹ in 0.5 M LiClO₄.

SL.1.4. Electropolymerization of PPyNPs on SPCE

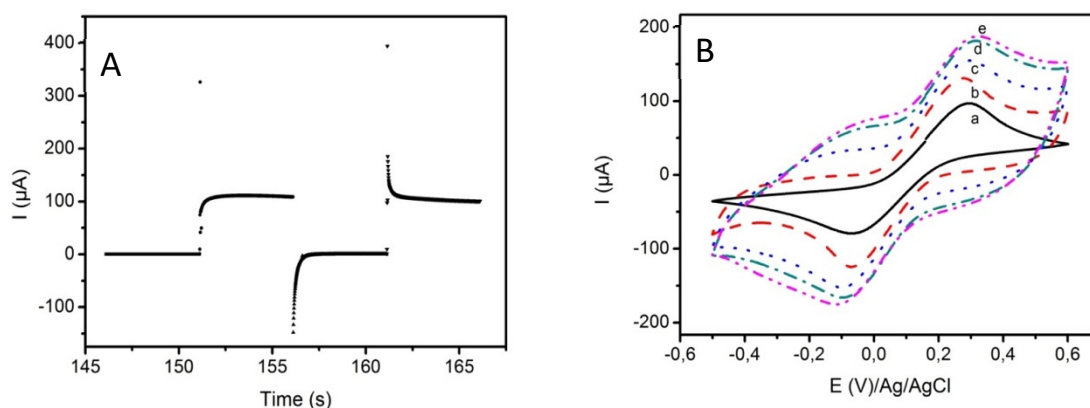


Figure S3. Electropolymerization of PPy by 2 pulses with $E_{app} = 0.8$ V during 5s in 0.5M LiClO₄ (A) CVs recorded in 5 mM [Fe(CN)₆]^{3/4-} at $v = 100$ mV.s⁻¹ before and after PPy electropolymerization (B.a) SPCE (B.b) 1 pulse (B.c) 2 pulses (B.d) 3 pluses and (B.e) 4 pulses

SL.1.5. Electrodeposition of EDA and Cystamine

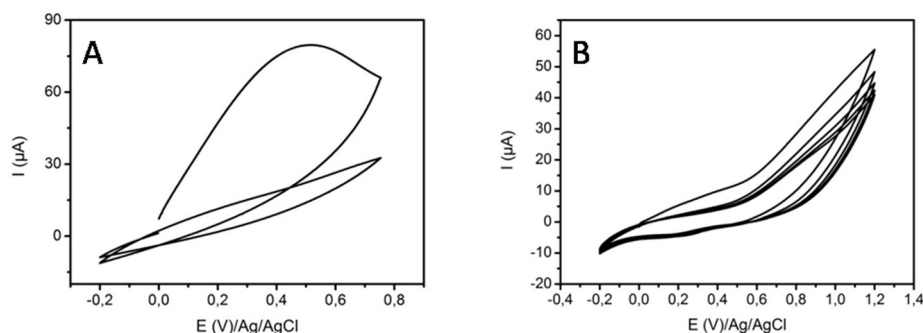


Figure S4. (A) CVs of Electrodeposition of EDA by cycling the potential between -0.2V and 0.8V, for 2cycles at scan rate 200 mV.s⁻¹, in 0.5 M LiClO₄, (B) Electrodeposition of Cystamine by cycling the potential between -0.2V and 1.2V, for 4 cycles at scan rate 100 mV/s, in 0.5 M LiClO₄

SI.2 Results and discussion

SI.2.1 Properties of MoS₂ and PPy

SI.2.1.1 Structural and morphological studies

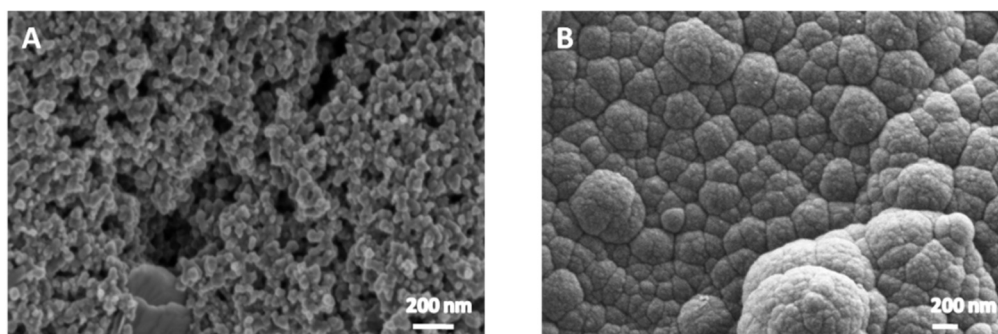


Figure S5. SEM images of (A) SPCE (B) SPCE/PPy Polypyrrole deposits using cyclic voltammetry

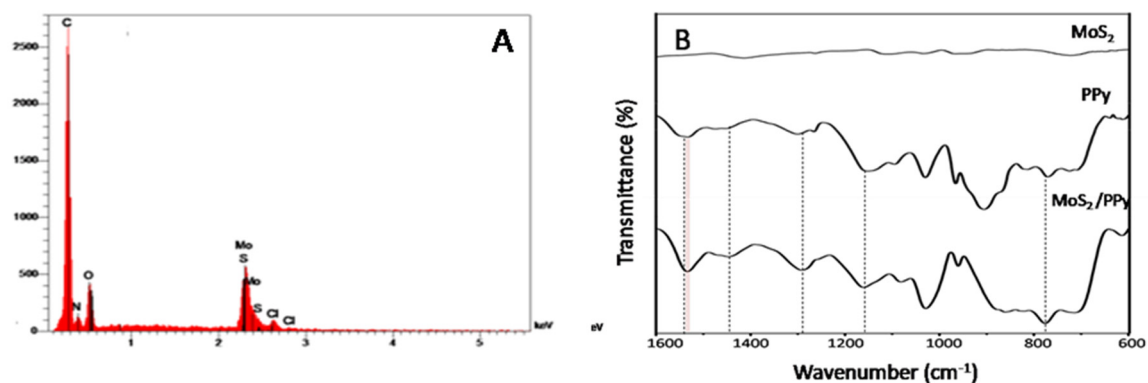
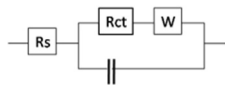
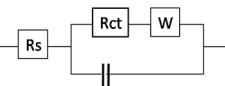
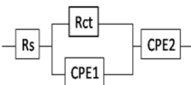
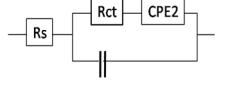


Figure S6. (A) EDX analysis of the modified SPCE with MoS₂/PPy and (B) FT-IR MoS₂ nanosheets, PPy and MoS₂/NPsPPy

SI.2.1.2. Electrochemical characterization of the nanocomposite

Table S1. Fitting parameters of EIS data

Equivalent circuit model	Modified electrode	R_s / Ω	R_{ct} / Ω	Capacitance μF	CPE1 μMho	n	CPE2 μMho	n	W μMho	χ^2
	SPCE	321.01	849.7	0.976	-	-	-	-	669	0.1
	SPCE/MoS ₂	316.7	411.61	1.19	-	-	-	-	1410	0.029
	SPCE/PPy	303.34	197.14	-	288	0.54	860	0.95	-	0.001
	SPCE/MoS ₂ /PPy	306.55		22.7	-	-	2190	0.634	-	0.01

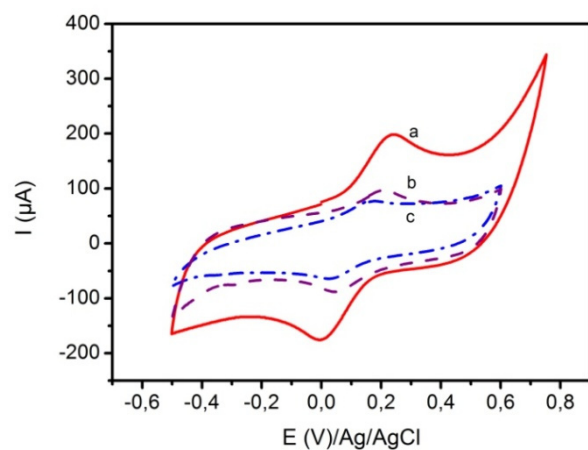


Figure S7. CVs recorded in presence of 5 mM $[\text{Fe}(\text{CN})_6]^{3/4-}$ (a) SPCE/MoS₂/PPy ; (b) SPCE/MoS₂/PPy/EDA ;(c) SPCE/MoS₂/PPy/EDA/NQ ;

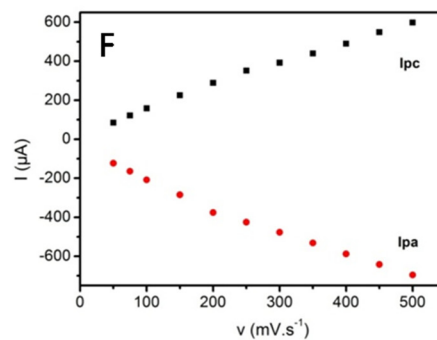
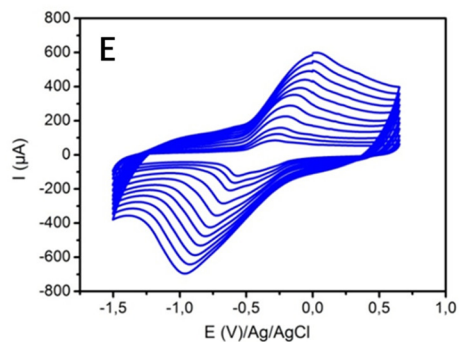
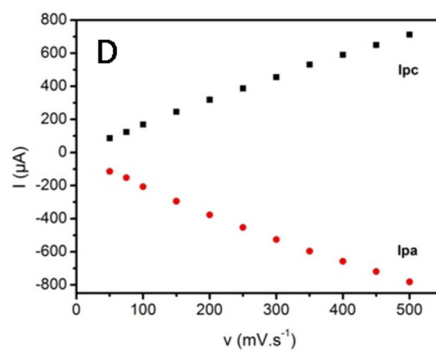
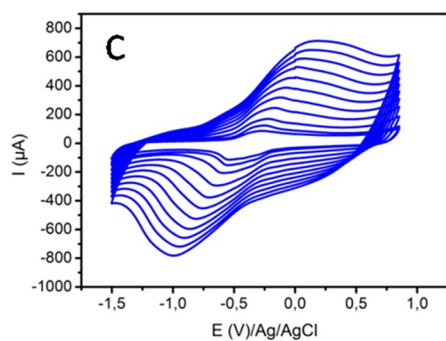
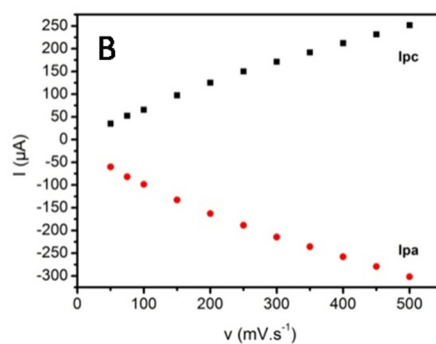
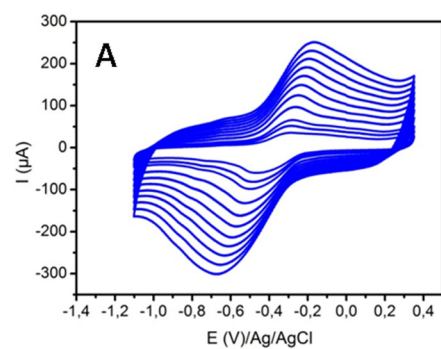


Figure S8. CVs of the redox signal of NQ in various modified SPCE in PBS pH= 7.4 with scan rate from 50 to 500 mV.s⁻¹ and Linear relationship of the redox peak currents versus scan rate (A, B) MoS₂/Cyst/NQ, (C, D) PPy/EDA/NQ, (E, F) MoS₂/PPy/EDA/NQ.

SI.2.2. Electrochemical characterization of the biolayers

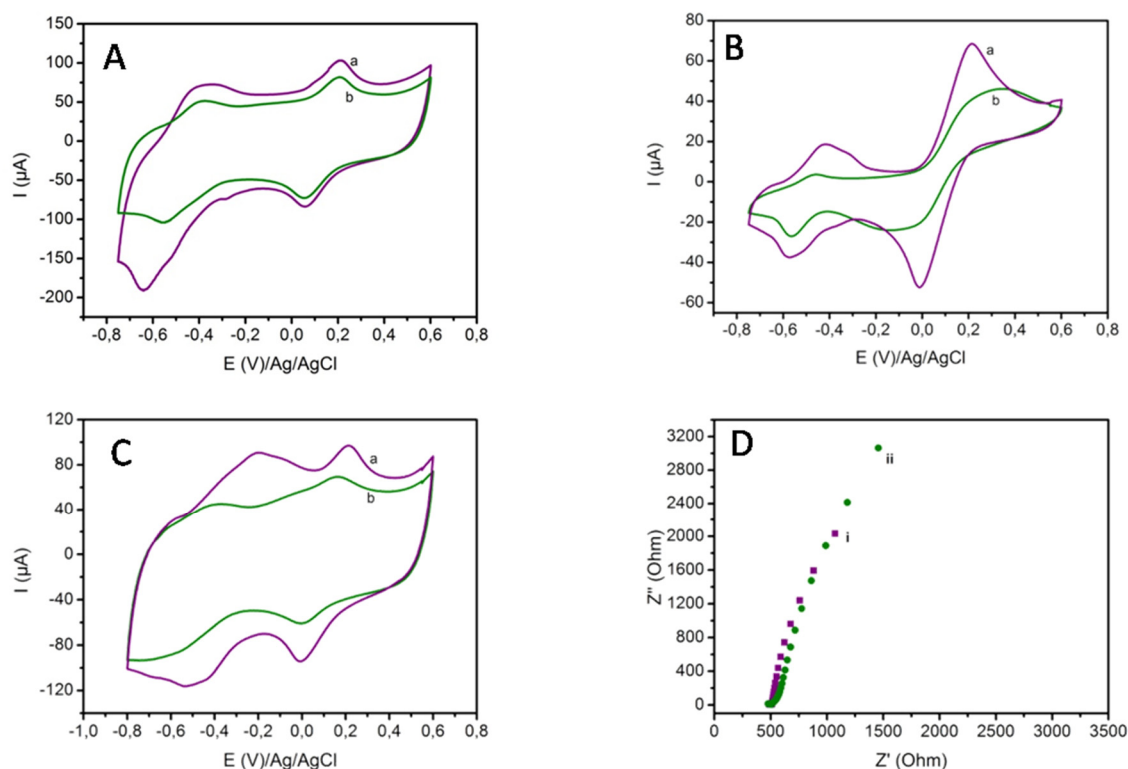


Figure S9. CVs recorded in presence of 5 mM [Fe(CN)₆]^{3/4-} before and after aptamer immobilization (A.a) SPCE/MoS₂/PPy/EDA/NQ; (A.b) SPCE/MoS₂/PPy/EDA/NQ/APT; (B.a) SPCE/MoS₂/Cyst/NQ, (B.b) SPCE/MoS₂/Cyst/NQ / APT; (C.a) SPCE/PPy/EDA/NQ; (C.b) SPCE/PPy/EDA/NQ/APT; EIS (Nyquist plots) in presence of 5 mM [Fe(CN)₆]^{3/4-} obtained before (D) (i) and after (D) (ii) aptamer immobilization (E_{app} = 0.2V) Frequency range: 100 KHz to 0.1 Hz.

SI.2.3. Comparison of sensing platforms based on MoS₂

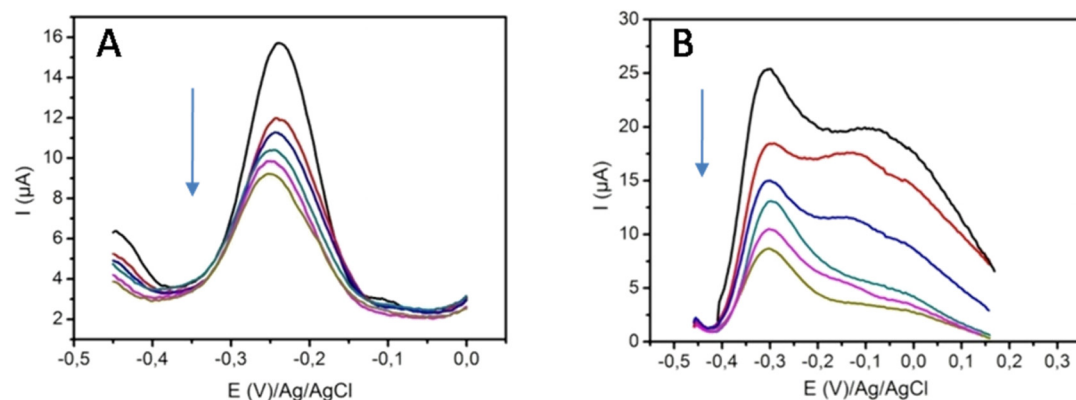


Figure S10. SWV of the oxidation peak after incubation at various ampicillin concentrations from 50 to 250 pg/L in PBS for (A) MoS₂ based electrode (B) PPy based electrode

SL.2.4. Detection in waste water

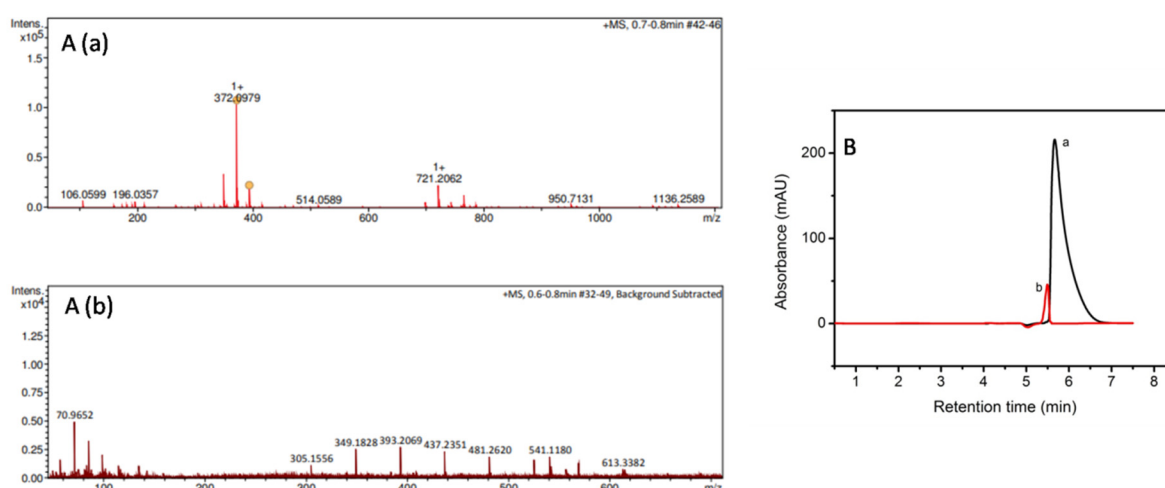


Figure S11. Mass Spectra of (a) water doped with AMP and (b) river water (B) High performance liquid chromatography (HPLC) analysis of (a) Ampicillin solution and (b) waste water sample