

## Electronic Supplementary Information

### **An electrochemical MIP sensors for selective detection of salbutamol based on a graphene/PEDOT:PSS modified screen-printed carbon electrode**

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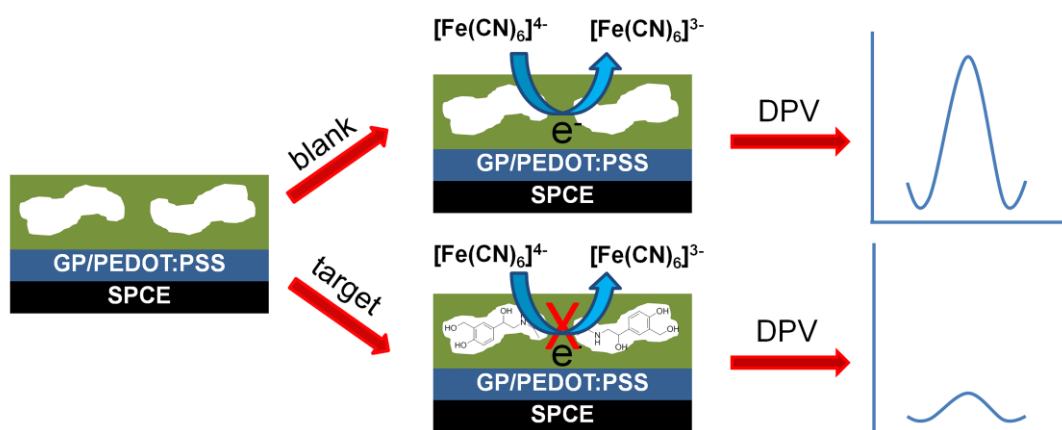
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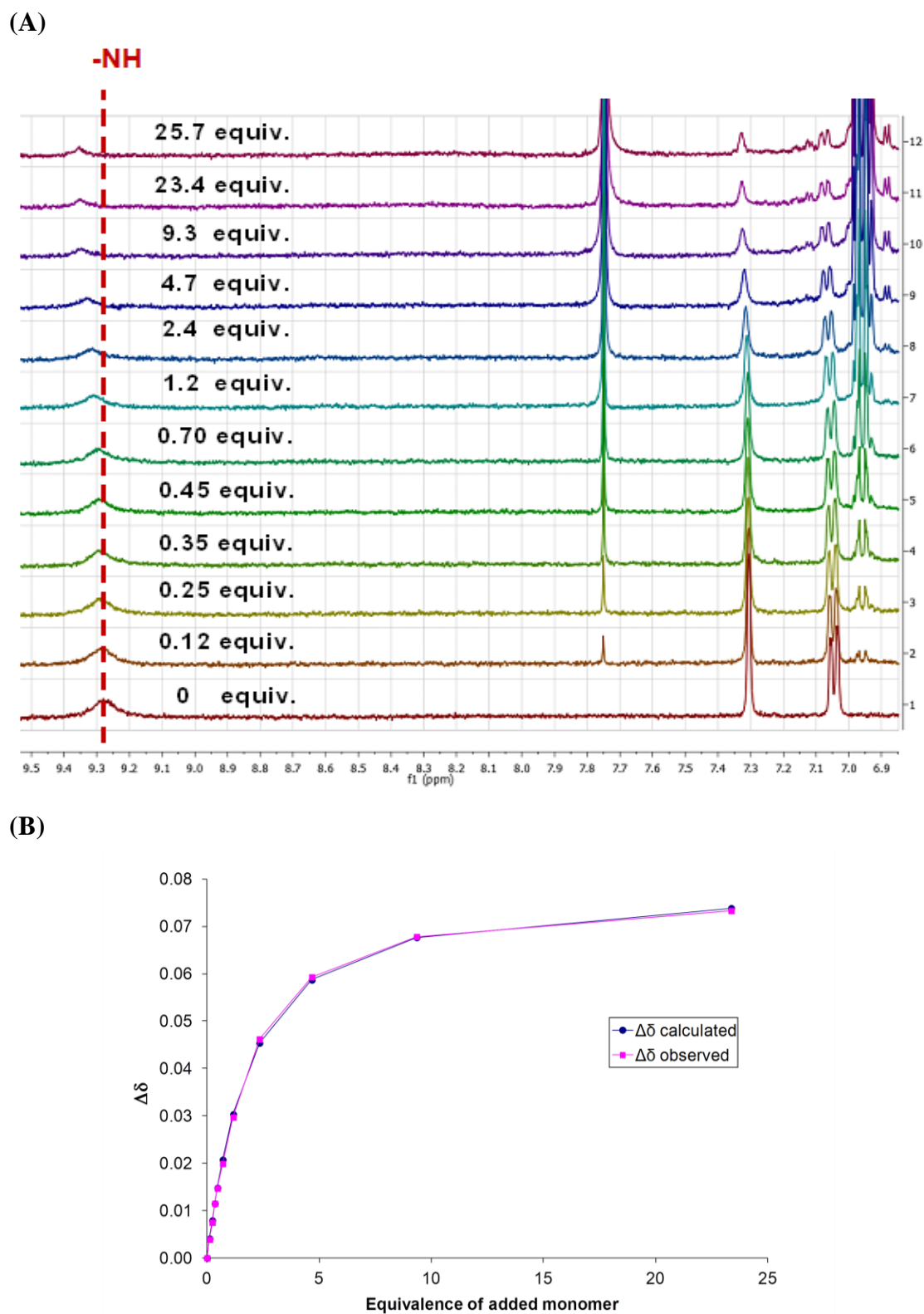
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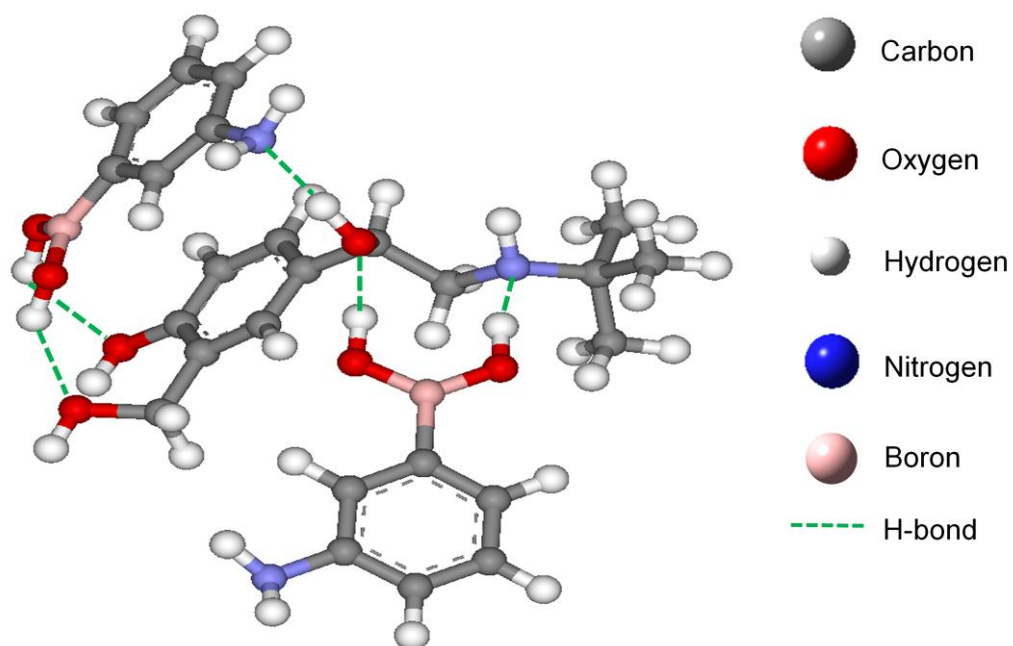
*E-mail address:* fscidcd@ku.ac.th



**Scheme S1** Schematic illustration for electrochemical determination of salbutamol using an electrochemical MIP sensor.

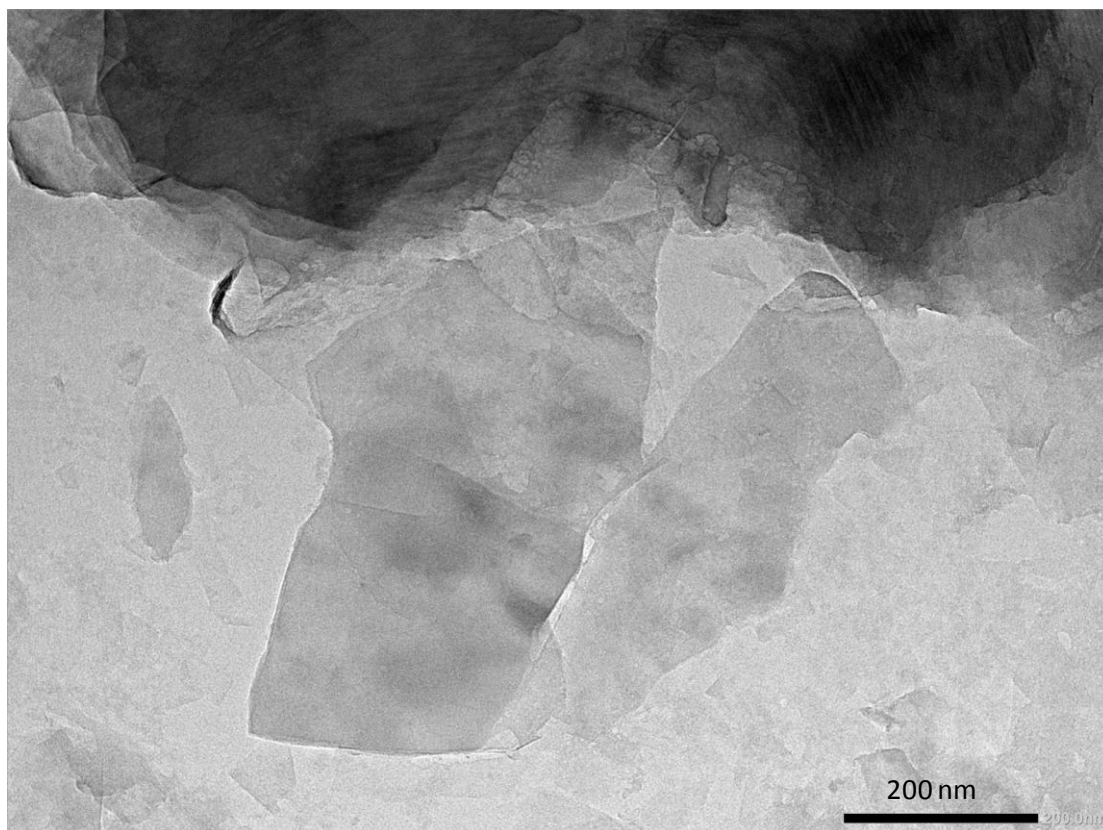


**Fig.S1** (A) Partial  $^1\text{H-NMR}$  spectra (500 MHz,  $\text{DMSO-d}_6$ ) from the titration of salbutamol with 3-aminophenylboronic acid. (B) Observed (magenta square) and calculated (blue circle) values for the  $^1\text{H-NMR}$  binding study of salbutamol and 3-aminophenylboronic acid.

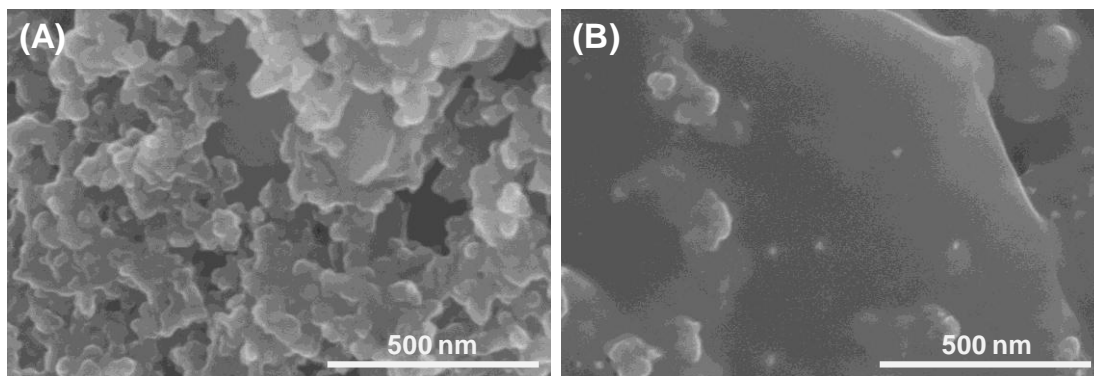


Interaction energy = -172.17883747 kJ/mol

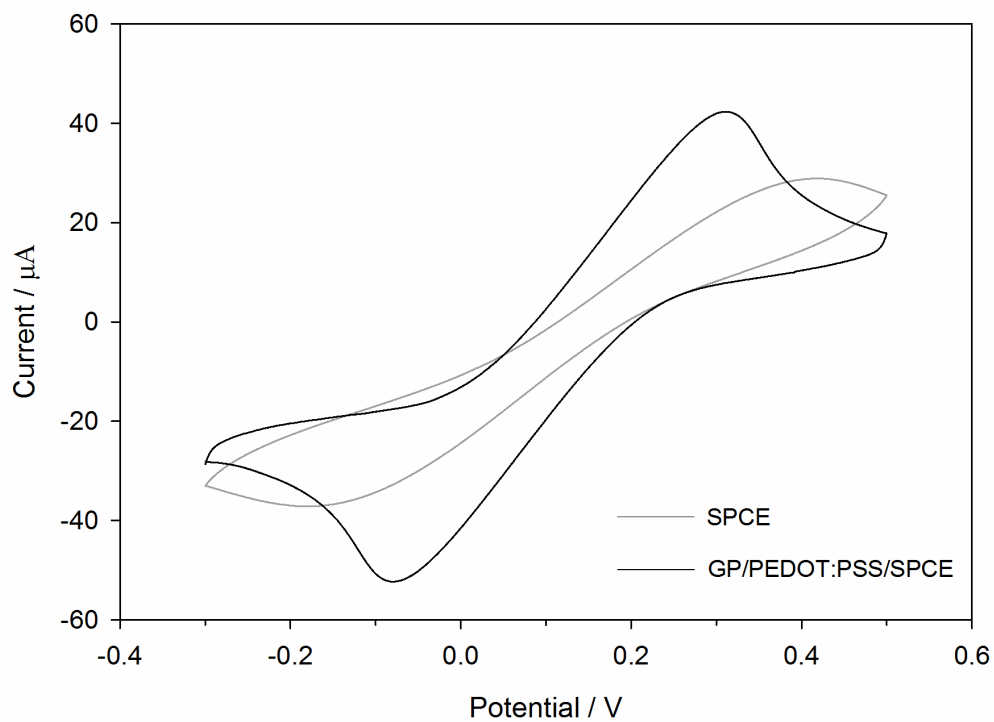
**Fig.S2** The optimized geometry of the possible salbutamol/aminophenylboronic acid complex and its interaction energy obtained by a computational simulation.



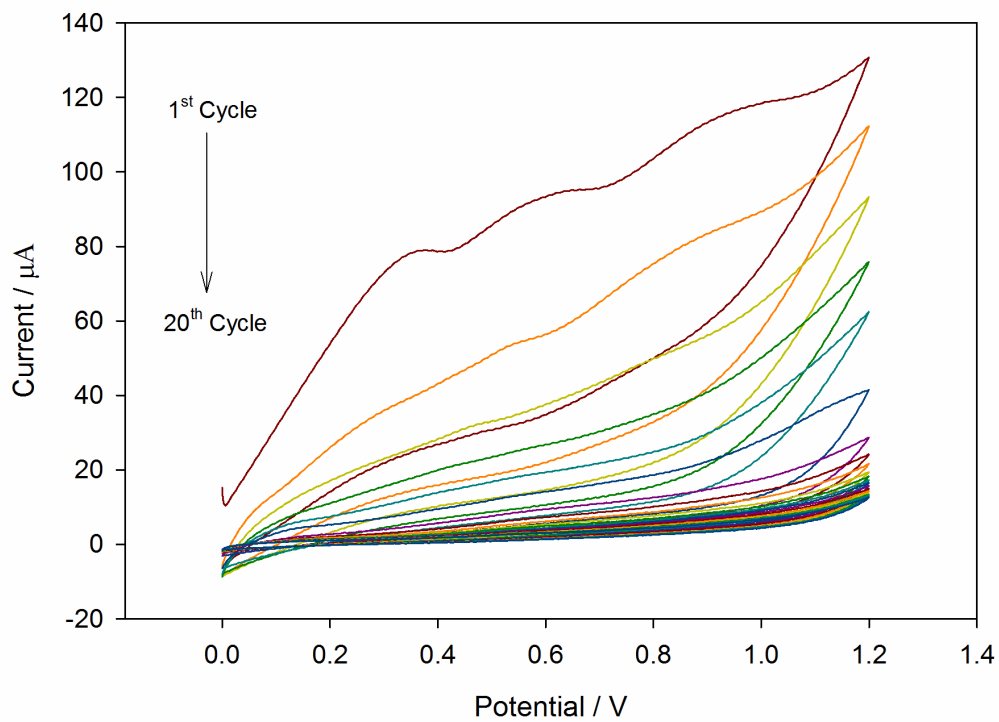
**Fig.S3** TEM image of graphene/PEDOT:PSS nanocomposite.



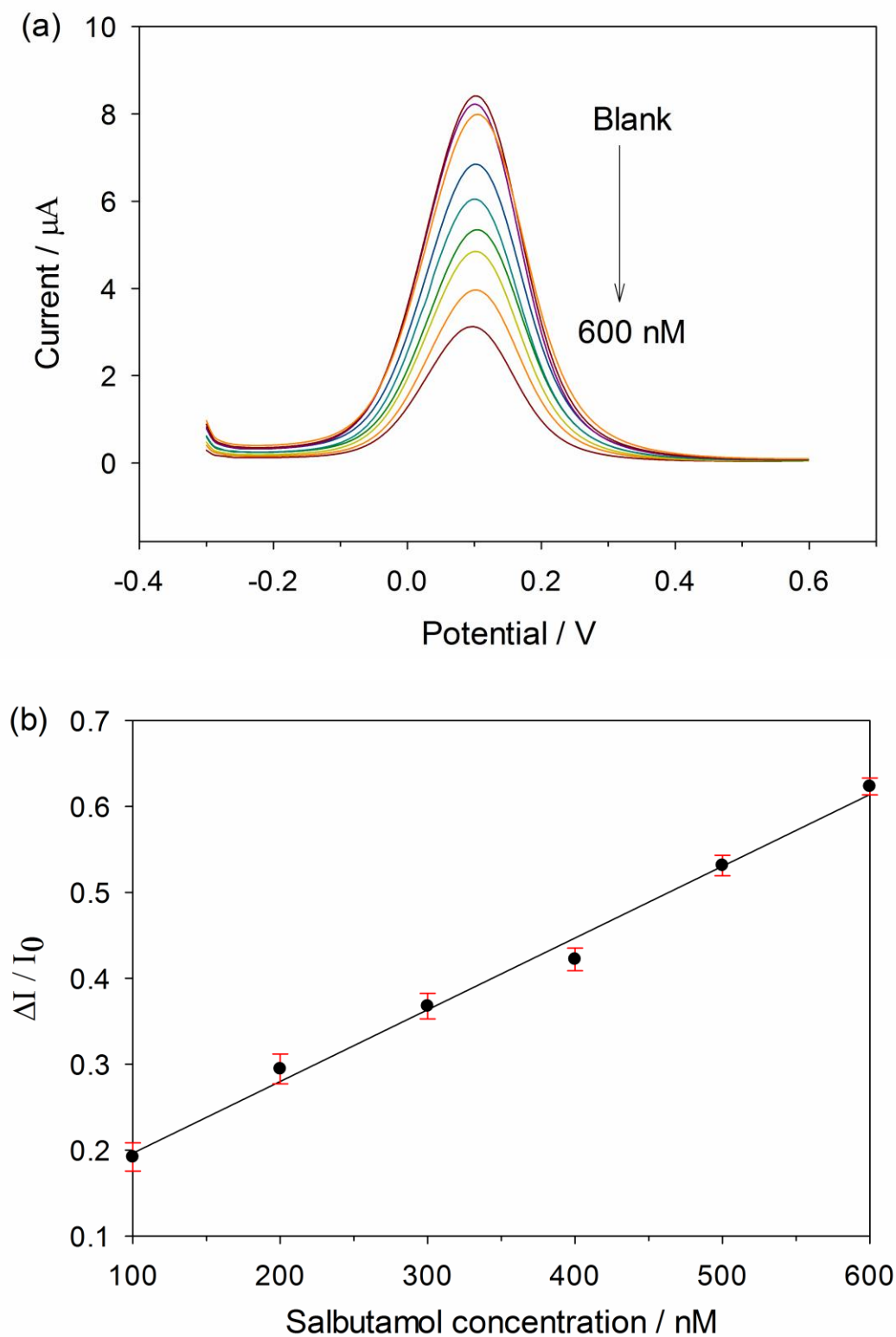
**Fig.S4** SEM images of (A) bare SPCE and (B) graphene/PEDOT:PSS modified SPCE.



**Fig.S5** Cyclic voltammograms of 5 mM K<sub>3</sub>[Fe(CN)<sub>6</sub>]/ K<sub>4</sub>[Fe(CN)<sub>6</sub>] in 100 mM KCl at bare SPCE and graphene/PEDOT:PSS modified SPCE.



**Fig.S6** Cyclic voltammograms for electrochemical polymerization of the imprinted film on graphene/PEDOT:PSS modified SPCE.



**Fig.S7** (a) Differential pulse voltammograms of MIP/SPCE recorded in 5 mM  $\text{K}_3[\text{Fe}(\text{CN})_6]/\text{K}_4[\text{Fe}(\text{CN})_6]$  after incubation in different concentrations of salbutamol, (b) Calibration curve of the MIP/SPCE. The error bars represent the standard deviation obtained from 6 independent measurements.

**Table S1** Association constants of the template molecule with monomers

<b>Template/Monomer</b>	<b><math>K_a</math> (<math>M^{-1}</math>)</b>
Salbutamol/3-Aminophenylboronic acid	$291 \pm 4\%$
Salbutamol/Scopoletin	$30 \pm 2\%$
Salbutamol/Resorcinol	$16 \pm 3\%$
Salbutamol/o-Phenylenediamine	- *

\* very small



**Table S2** Comparison of reported electrochemical sensors for the determination of salbutamol

Electrode material	Detection method	LOD	Linear range	Reference
GP-PEDOT:PSS/SCPE	CV	1.25 $\mu$ M	5 $\mu$ M – 550 $\mu$ M	[1]
NG/ITO	SWV	260 nM	0.17 $\mu$ M – 6.9 $\mu$ M	[2]
MnO <sub>2</sub> /RGO@NF	DPV	23 nM	42 nM – 1.46 $\mu$ M	[3]
ZrO <sub>2</sub> -polytaurine/GCE	LSV	20 nM	5 $\mu$ M – 220 $\mu$ M	[4]
AuNP/GCE	DPSV	20 nM	17 nM – 520 nM	[5]
Poly-ACBK/GO-nafion/GCE	LSV	4.8 nM	7 nM – 125 nM	[6]
Fe <sub>2</sub> TiO <sub>5</sub> - CPE	DPAdSV	90 pM	0.2 nM – 25 nM	[7]
Ab-AgPdNPs/Ab-rGO	LSV	4.8 pM	35 pM – 350 nM	[8]
Aptamer/Au	DPA	1.7 pM	0.35 pM – 35 pM	[9]
<b>MIP</b> membrane/SPE	Conductometry	13.5 nM	50 nM – 280 nM	[10]
<b>MIP</b> /Ag-N-RGO/GCE	DPV	7 nM	30 nM – 20 $\mu$ M	[11]
<b>MIP</b> /SWNTs/GCE	DPV	3 nM	10 nM – 830 nM	[12]
<b>MIPNP</b> -CPE	DPV	0.6 nM	1 nM – 55 nM	[13]
<b>MIP</b> /GP-PEDOT:PSS/SPCE	DPV	0.1 nM	1 nM – 1.2 $\mu$ M	This work

Ab: antibody, AgPdNPs: silver-palladium alloy nanoparticle, CS: chitosan, GCE: glassy carbon electrode, CPE: carbon paste electrode, DPAdSV: differential pulse adsorptive stripping voltammetry, DPSV: differential pulse stripping voltammetry, GP: graphene, LSV: linear sweep voltammetry, MIPNP: imprinted nanoparticle, MWNTs: multi-walled carbon nanotubes, NF: nickel foam, NG: nano gold, N-RGO: nitrogen doped reduced graphene oxide, Poly-ACBK: poly(acid chrome blue K), SPE: screen printed electrode, SPCE: screen printed carbon electrode, SWNTs: single walled carbon nanotubes, SWV: square wave voltammetry

**Table S3** Comparison for determination of salbutamol in real samples using HPLC and the established sensor.

Method	Feed sample			Swine meat		
	Spiked (nM)	Found (nM)	Recovery (%)	Spiked (nM)	Found (nM)	Recovery (%)
This work	1,000	990	99.0	1,000	1,027	102.7
HPLC	1,000	1,011	101.1	1,000	1,034	103.4

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