New journal of chemistry

Fabrication of sensitive silver-decorated cotton swabs for SERS quantitative detection of mixed pesticide residues in bitter gourds

Lili Kong,[a] Meizhen Huang,*[ab] Jie Chen [a] and Mengshi Lin [c]

a. Department of instrument Science and Engineering, Shanghai Jiao Tong University, Shanghai 200240, China. Email: mzhuang@sjtu.edu.cn

b. Shanghai Research Center of Engineering and Technology for Inteligent Diaginosis and Treatment Instrumentation, Shanghai Jiao Tong University, Shanghai 200240, China

c. Food Science Program, Division of Food Systems & Bioengineering, University of Missouri, Columbia, Mo 65211, USA

List of supplementary material

SI-1 Estimated amount of AgNPs coated on a cotton swab

The amount of AgNPs on a cotton swab (m_{Ag}) could be calculated according to the following formula:

$$m_{Ag} = C_{AgNO_3} \cdot V_{AgNO_3} \cdot M_{Ag} \cdot \frac{0.75\ ml}{100\ ml}$$

Where C_{AgNO_3} is the molarity of $AgNO_3$, $V_{AgNO_3}$is the volume of $AgNO_3$ solution, and M_{Ag} is the relative molecular mass of Ag. m_{Ag} is calculated to be 8.09×10^{-2} mg. Actually, considering the loss of reduction efficiency and modification efficiency, the amount of AgNPs attached on a cotton swab is less than 8.09×10^{-2} mg.

SI-2 Mechanism of NaCl facilitated decoration process

The main component of cotton swab is cellulose, which contains abundant uronic acid groups, making cotton swab negatively charged.[S1] While AgNPs are also negatively charged.[S2] The presence of electrostatic repulsion makes it difficult to decorate AgNPs on cotton swabs by immersion adsorption. The introduction of NaCl can break the electrostatic repulsion and accelerate the decoration process, because NaCl has a strong attraction on AgNPs.[S3]

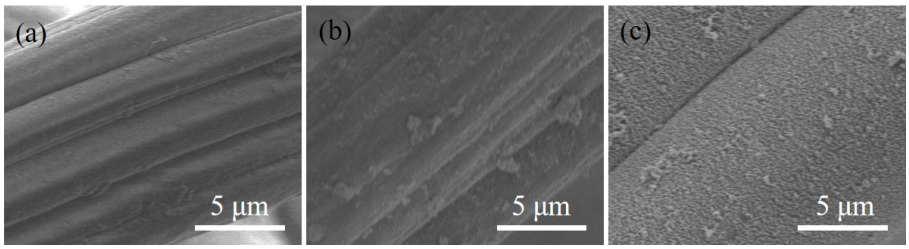

Figure S1 (a) SEM images of blank cotton swab, (b) silver-decorated cotton swabs without NaCl treatment and (c) with NaCl treatment.

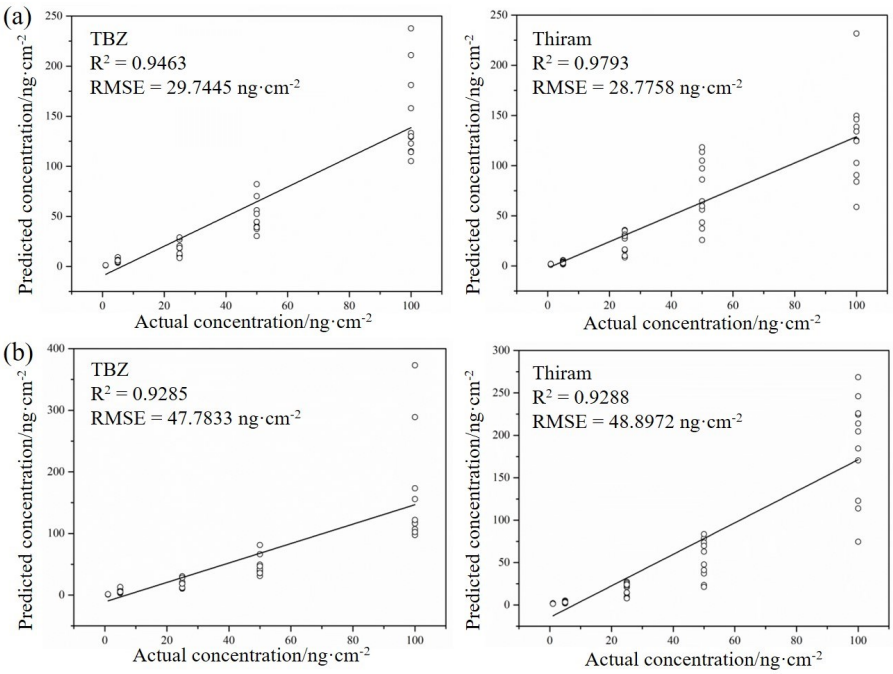

Figure S2 (a) Predicted concentrations compared with actual concentrations of TBZ and thiram in bitter gourds using ULR models and (b) PCR models.

Table S1 Vibration assignments of R6G[S4]

Raman shift/cm^{-1}	Vibrational mode
771	C–H out-of-plane bending
1182	C–H in-plane bending
1311	N–H in plane bending
1362, 1511	Aromatic C–C stretching

Table S2 Vibration assignments of TBZ and thiram[S5, S6]

Raman shift/cm^{-1}	Vibrational mode	Material assignment
783	Out of plane bending of C-H	TBZ
884, 900	Out of plane bending of C-H and C-C-C deformable vibration	TBZ
1010	Out of plane bending of C-C-C	TBZ
561	S-S stretching	Thiram
925	C=S stretching	Thiram
1147	Methyl vibration	Thiram
1381	Methyl or C-N stretching	Thiram
1507	Methyl vibration	Thiram

References

[S1] Y. V. Sood, R. Tyagi, S. Tyagi, P. C. Pande and R. Tondon, *J. Sci. Ind. Res. India*, 2010, **69**, 300-304.

[S2] P. Liou, F. X. Nayigiziki, F. Kong, A. Mustapha and M. Lin, *Carbohyd. Polym.*, 2017, **157**, 643-650.

[S3] M. Kim and K. Itoh, *J. Phys. Chem.*, 1987, **91**, 126-131.

[S4] Y. Wang, S. Ma, Q. Yang and X. Li, *Appl. Surf. Sci.*, 2012, **258**, 5881-5885.

[S5] K. Wang, X. Zhang, C. Niu and Y. Wang, *ACS Appl. Mater. Inter.*, 2014, **6**, 1272-1278.

[S6] P. Nie, T. Dong, S. Xiao, L. Lin, Y. He and F. Qu, *Molecules*, 2018, **23**, 1949.