Electronic Supplementary Material (ESI) for Analyst.
This journal is © The Royal Society of Chemistry 2019

Supplementary Information

Monitoring 2,3',5,5'-tetrachlorobiphenyl with rapid and sensitive environmental aptamer sensor

Siyao Siyao Liu,‡[a,b], Qianqian Chen,‡[a,b], Zhiming Wang[b], Tongcheng Cao[*b], Guohua Zhao[*b] and Yongxin Zhou[*a]

[a] Department of Cardio-Thoracic Surgery, Institute of Translational Research, Tongji Hospital, Tongji University School of medicine, Shanghai 200065, People's Republic of China

[b] School of Chemical Science and Engineering, Tongji University, Shanghai 200092, People's Republic of China

* Corresponding author: Tongcheng Cao, Guohua Zhao, Yongxin Zhou

E-mail: ctc@tongji.edu.cn, g.zhao@tongji.edu.cn, zhou6302@tongji.edu.cn

‡ These authors are co-first authors and contributed equally to this work.

Supplementary Methods and Data

S1. Design and preparation of SERS substrate.

Gold nanoparticles were prepared by reduction of gold (III) chloride hydrate using trisodium citrate. To be specific, 100 mL 0.01% (w/w) $HAuCl_4 \cdot 3H_2O$ was reduced by 1.5 mL 1% (w/w) trisodium citrate solution at 100 °C under vigorous magnetic stirring for 15-20 min until the solution turned from colorless to wine red. The as-prepared wine red-colored Au particles were used as seed particles. Then 800 μL of $AgNO_3$ solution (0.5%, w/w) was added to 100 mL of boiling gold seed solution. Afterwards, 1 mL of sodium citrate solution (1%, w/w) was used as the reducing agent and added dropwise with stirring. The solution was boiled for 1 h, then cooled down to room temperature. The Au@Ag NPs were thus obtained and stored in the refrigerator at 4℃.

S2. The process of PCB72 detection.

The final concentration range of PCB72 was from 0 to 1000 pg/mL. The measurement was chosen 20× objective lens to focus a laser spot. The collecting parameters of each SERS spectrum were exposures time of 5 s and integrating twice over a spectral range from 800 cm^{-1} to 1800 cm^{-1}.

S3. Molecular docking simulation.

With the development of computer technology, molecular docking simulation technology has been widely used to study the conformation and free energy calculations between receptors and ligands, and used to study the mechanism of reaction and binding between molecules.[1] The molecular docking simulation method

is mainly to place the small molecule ligand at the active site of the macromolecular receptor. The AutoDock[2] written by Olsen of the Scripps Research Institute can be effectively applied to docking between receptors and ligand molecules, and is a relatively high-accuracy docking software.

Running AutoDock requires predicting the 3D structure of aptamers and target molecules. The proposed RNA Composer[3] is a user-friendly, free-for-use predictor of RNA 3D structure (http://rnacomposer.ibch.poznan.pl) which is based on the sequence of aptamers (or two-dimensional structure) to predict its 3D structure. To predict the three-dimensional structure of DNA, we tried to predict the 3D structure of a DNA aptamer by using the means of predicting the 3D structure of RNA. It was necessary to prepare U-uracil for replacing the base T-thymine in the DNA aptamer. And it was assumed that there is no change in the 3D structure of the aptamer after changing the base. The 3D structure of contaminants was obtained by Chemoffice, mainly used Chemdraw in Chemoffice to draw necessary chemical structures, and then copied the graphic structure into Chem3D.

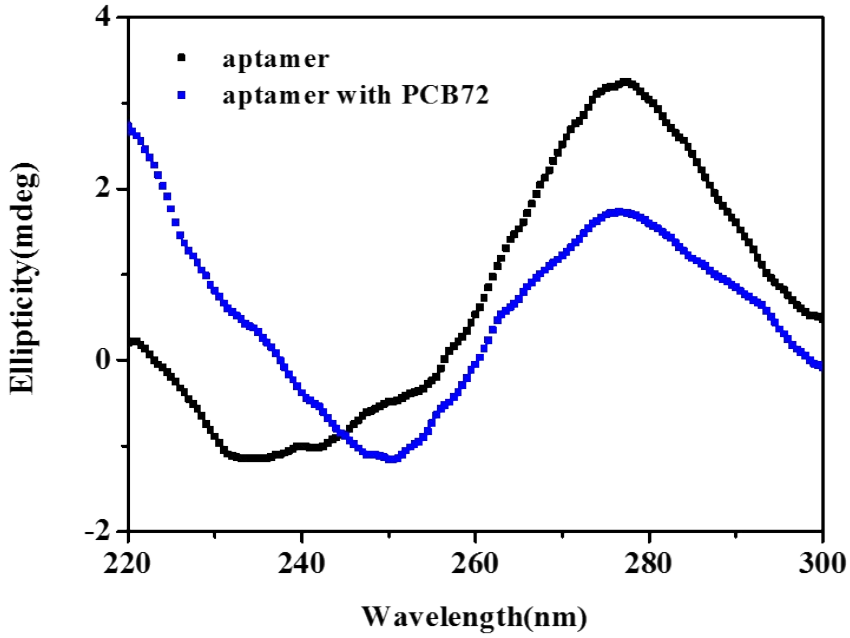

Fig. S1. Circular dichroism spectroscopy of aptamers (4μM) in the absent and present PCB72.

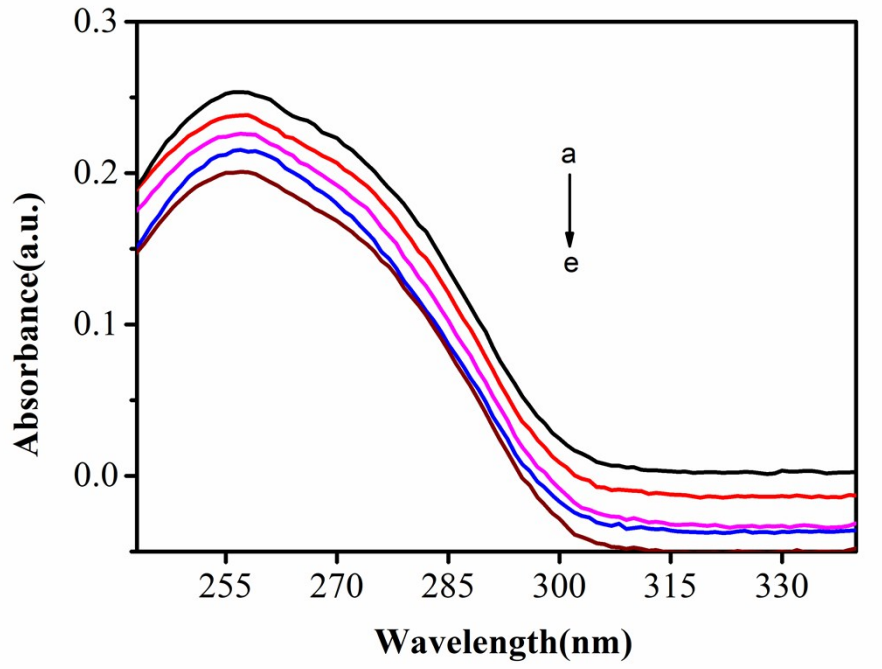

Fig. S2. UV absorbance spectra of aptamers (2 μM) with PCB72 concentration (a-e: PCB72 concentrations are 0, 0.5 μM, 1 μM, 1.5 μM and 2 μM).

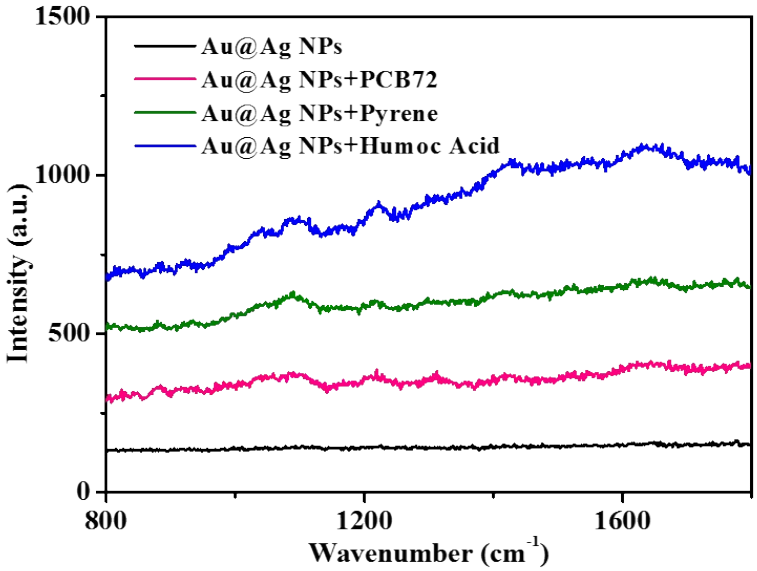

Fig. S3. The SERS signal of different pollutants interacting with Au@Ag NPs.

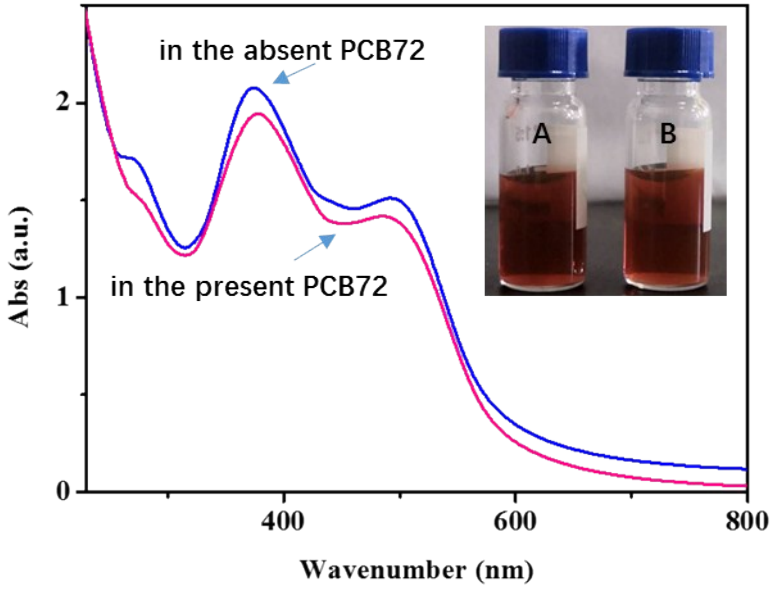

Fig. S4. UV–vis spectra of Au@Ag NPs modified with 4MBA in the absent and present PCB72. Inset is the Au@Ag NP aqueous solutions before (A) and after (B) PCB sensing.

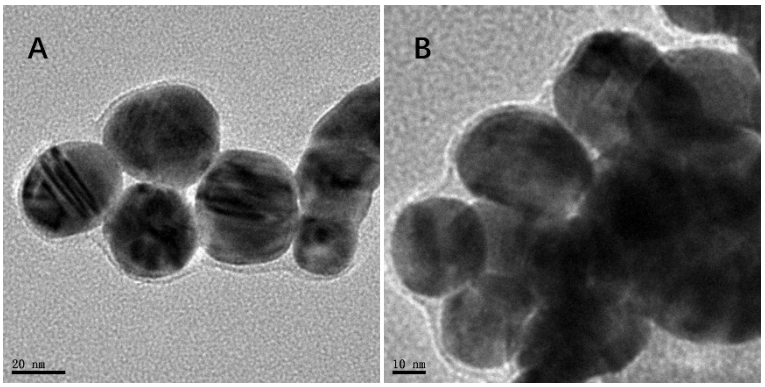

Fig. S5. HRTEM image of Au@Ag NPs modified with 4MBA before (A) and after the add of PCB72 (B), respectively.

Table S1. *P*-valus of the different of interferences in comparison to PCB72(**P*<0.05, ***P*<0.01 and ****P*<0.001).

Interference	PCB77	PCB101	PCB126	Atrazine	Bisphenol A	Naphthalene	Pyrene	Humic Acid
P value	0.000019	0.000005	0.000006	0.000008	0.000005	0.000006	0.000011	0.000007

References

1. N. El-Hachem, B. Haibe-Kains, A. Khalil, F. H. Kobeissy and G. Nemer, in Neuroproteomics, Springer, 2017, pp. 391-403.
2. S. Cosconati, S. Forli, A. L. Perryman, R. Harris, D. S. Goodsell and A. J. Olson, Expert opinion on drug discovery, 2010, 5, 597-607.
3. M. Biesiada, K. Pachulska-Wieczorek, R. W. Adamiak and K. J. Purzycka, Methods, 2016, 103, 120-127.