Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information:

A label-free RTP sensors based on aptamer/quantum dots nanocomposites for cytochrome c detection

Dongxia Li*, Junping Guo, Liang Zhao, Guoxian Zhang, Guiqin Yan*

Shanxi Normal University, Linfen 041004, PR China

*Corresponding authors.
E-mail addresses: lidx_139@163.com (D, Li), gqyan2013@163.com (G. Yan)

Table S1 Comparison of different optical sensors in Cyt c detection

Materials	Methods	Linear Range	Detection Limit	Reference
CdTe QDs	Label-free fluorescence turn off	0.5-2.5 μM	0.5 μM	49
N-GQDs@MIP	Label-free fluorescence turn off	0.2-60 μM	0.11 μM	12
UCNPs@MIP	Label-free fluorescence turn off	1-24 μM	0.73 μM	13
CdTe QDs@MIP	Label-free fluorescence turn off	0.97-24 μM	0.41 μM	14
Cy5-aptamer/GO	Label fluorescence turn on	0.03-10 μM	0.01 μM	50
TAMRA-aptamer/AuNPS	Label fluorescence turn on	0.1-10 μM	0.0167 μM	51
Aptamer/Mn-ZnS QDs	Label-free Phosphorescence turn off	0.166-9.96 μM	0.084 μM	This work

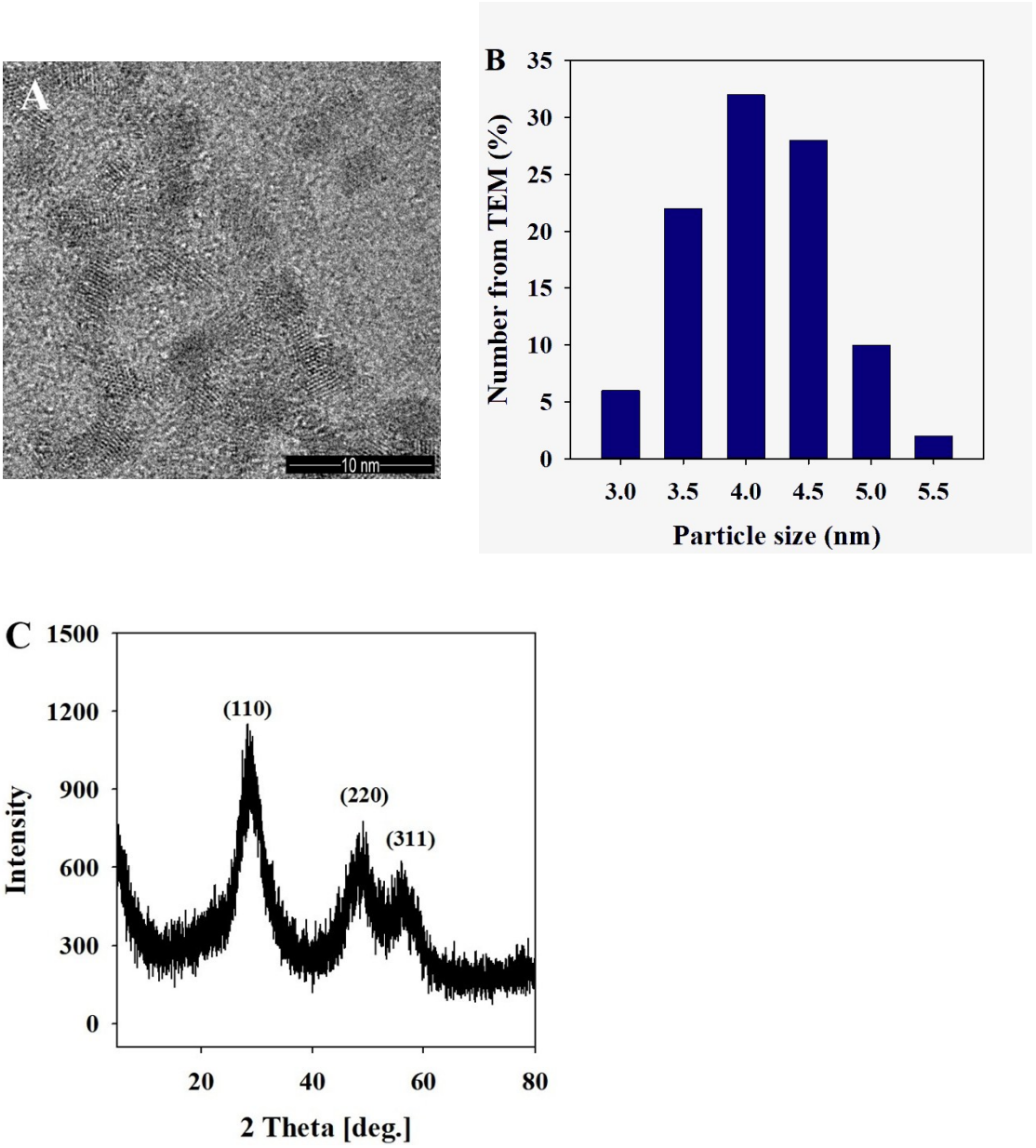

Fig. S1 (A)TEM image of PEI-QDs; (B) Size distribution of PEI-QDs in diameter; (C) XRD images of PEI-QDs.

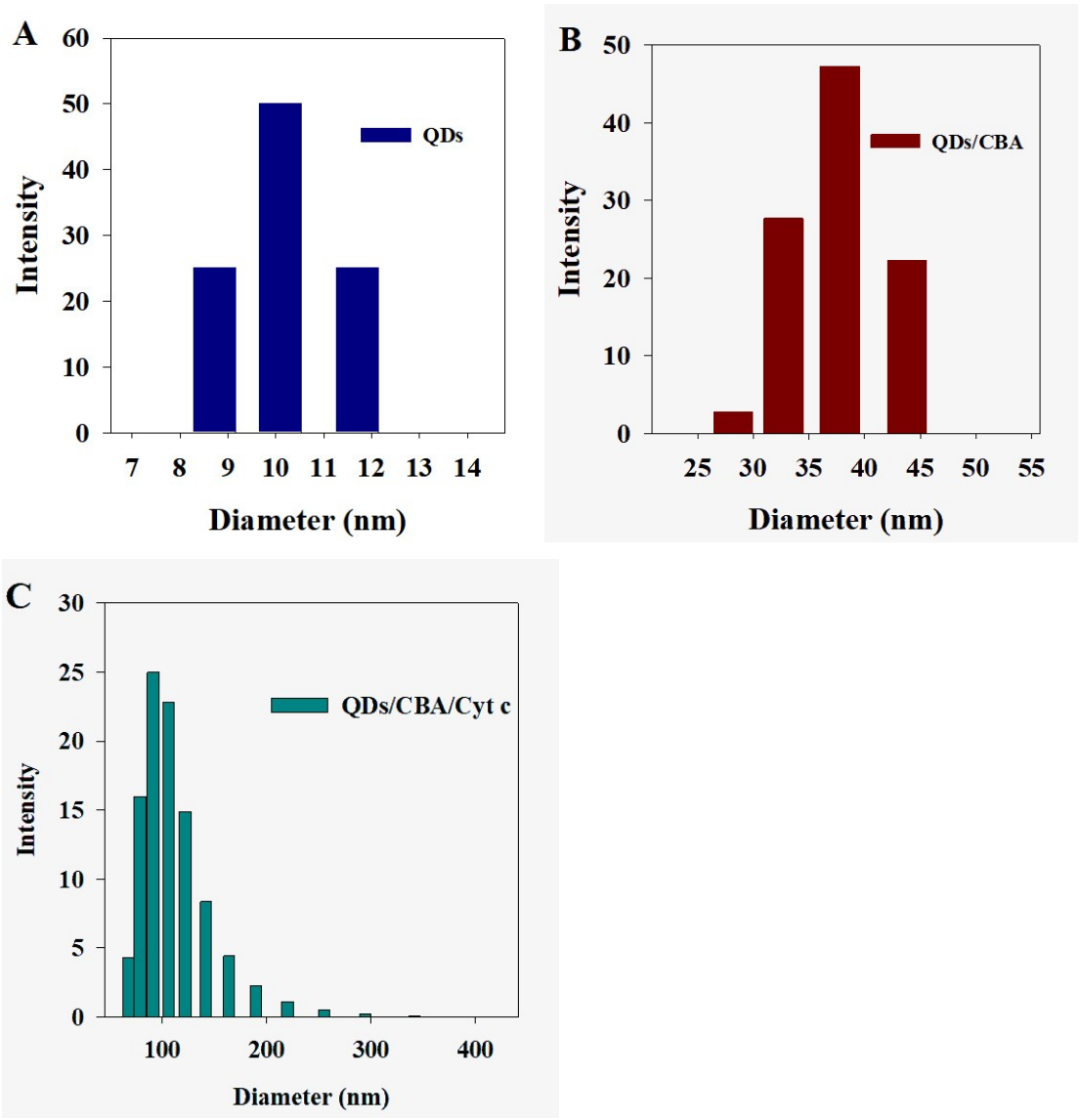

Fig. S2 DLS measurement of PEI-QDs (A), QDs/CBA (B) and QDs/CBA/Cyt c (C).

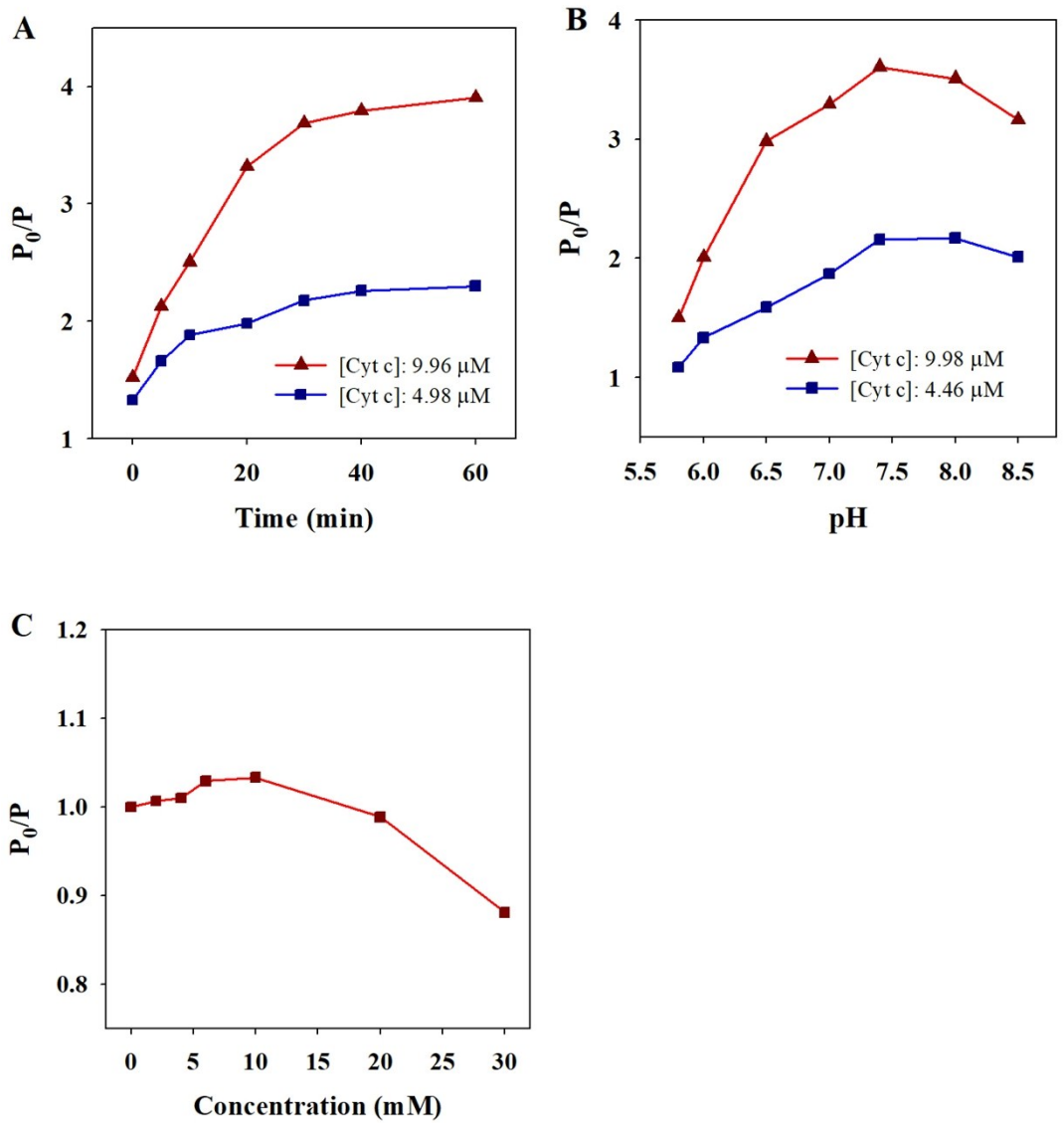

Fig. S3 (A) The effect of incubation time on the responses of QDs/CBA to Cyt c; (B) The effect of pH on the responses of the QDs/CBA to Cyt c; (C) The effect of NaCl concentration on the responses of QDs/CBA to Cyt c. P_0 and P represent the RTP intensity of the QDs/CBA nanocomposites before and after incubation with Cyt c.

Molecular docking analysis

1. Molecular docking procedure

Molecular docking were performed to investigate the binding mode between the Bos taurus Cyt c to the CBD (Cyt c aptamer: 5'-ATC GAT AAG CTT CCA GAG CCG TGT CTG GGG CCG ACC GGC GCA TTG GGT ACG TTG TTG CCG TAG AAT TCC TGC AGC C-3') using the Hex version 8.0.0 (http://hex.loria.fr/). The three-dimensional (3D) structure of the Cyt c (PDB ID: 2B4Z) was downloaded from Protein Data Bank,[1] while the 3D structure of the single stranded DNA was built by SYBYL-X 2.0 package.[2] For docking, the default parameters were used as described in the Hex. The top ranked pose as judged by the docking score was subject to visually analyze using PyMoL 1.7.6 software.

2. Docking results analysis

To research the action mode of cyt c and Cyt c aptamer from the molecular perspective, we docked the Cyt c to its binding pocket of aptamer. Detailed analysis showed that a hydrophobic interaction was observed between the residues Ala-51 and Pro-76 of the Cyt c and the nucleotides DT-44, DG-45 and DG-46 of the CBA. The residues Lys-73 and Lys-87 of the Cyt c formed cation-π interactions with the nucleotides DA-42 and DC-36 of the CBA, respectively, whereas the residue Lys-13 of the Cyt c formed cation-π interactions with the nucleotides DG-37 and DG-38 of the CBA. In addition, anion-π interactions were observed between the residue Glu-90 of the Cyt c and the nucleotides DC-36 and DG-37 of the CBA. Importantly, four

hydrogen bond interactions were shown between the residue Lys-73 of the Cyt c and the DA-42 of the CBA (bond length: 1.9 Å), the Gly-84 of the Cyt c and the DC-39 of the CBA (bond length: 1.5 Å), the Lys-86 and Lys-13 of the Cyt c and the DG-38 of the CBA (bond length: 1.7 and 2.1 Å), which were the main binding affinity between the Cyt c and the CBA.

In conclusion, the above molecular simulations give us rational explanation of interactions between the Cyt c and the Cyt c aptamer.

References

1. N. Mirkin, J. Jaconcic, V. Stojanoff and A. Moreno, *Proteins*, 2008, 70, 83-92.
2. G. M. Morris, R. Huey, W. Lindstrom, M. F. Sanner, R. K. Belew, D. S. Goodsell and A. J. Olson, *J. Comput. Chem.*, 2009, 30, 2785-2791.