Supplementary Information

An aptamer-based fluorescence probe for facile detection of lipopolysaccharide in drink

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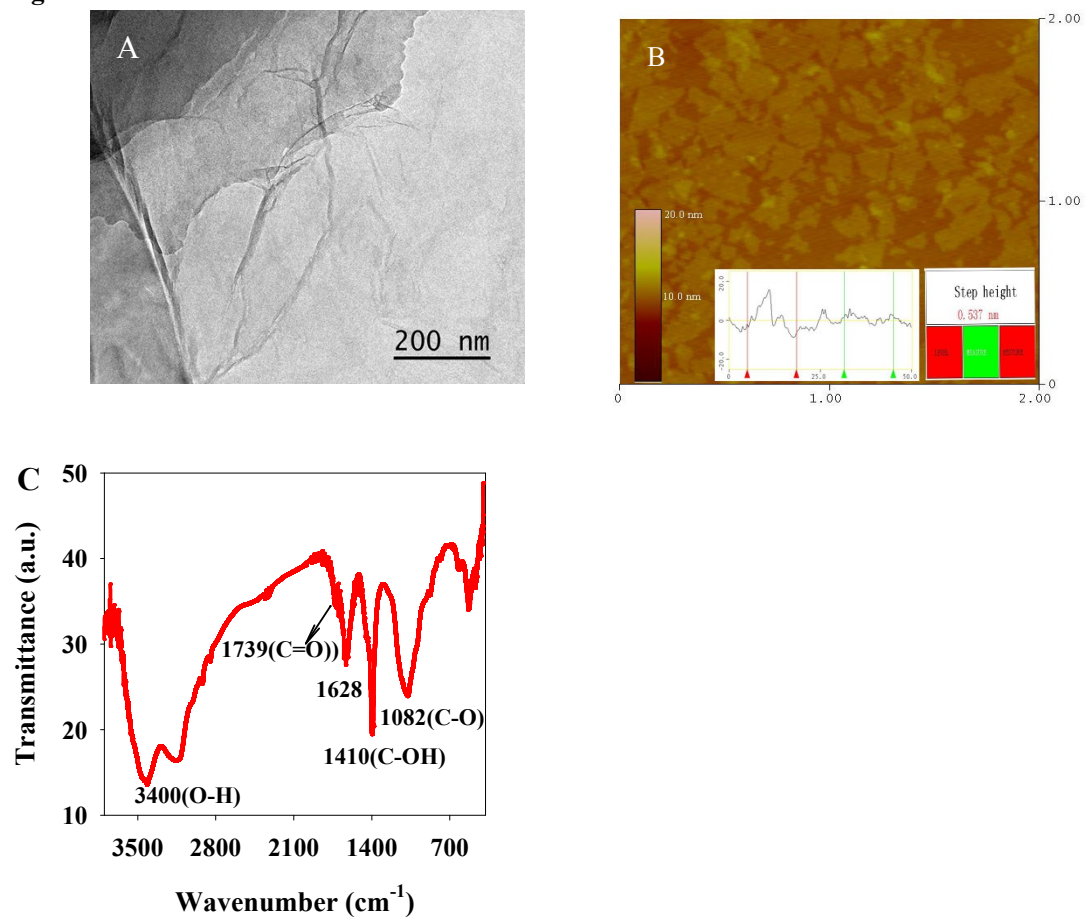*Corresponding author. Fax: (86) 0357-2051243. E-mail: zzfsx2012@126.com.

Fig.S1.

Fig.S1. (A) HRTEM images of GO. **(B)** AFM images of GO. **(C)** FT-IR spectra of GO.

Fig.S2.

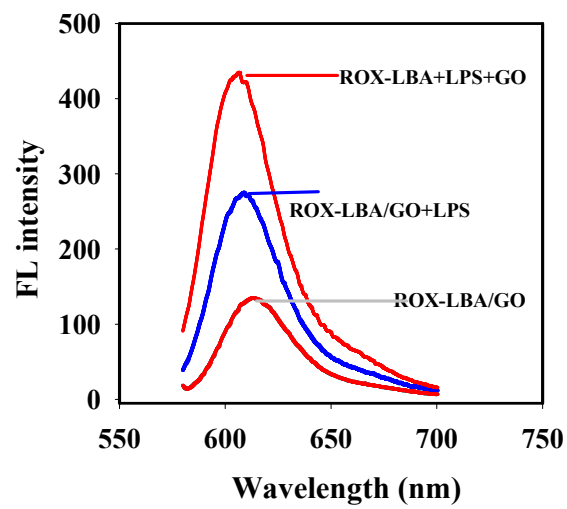**Fig.S2.** The effect of adding order of LPS on the sensing system. The concentration of LPS and GO was 800 ng mL^{-1} and 30 μg mL^{-1}.
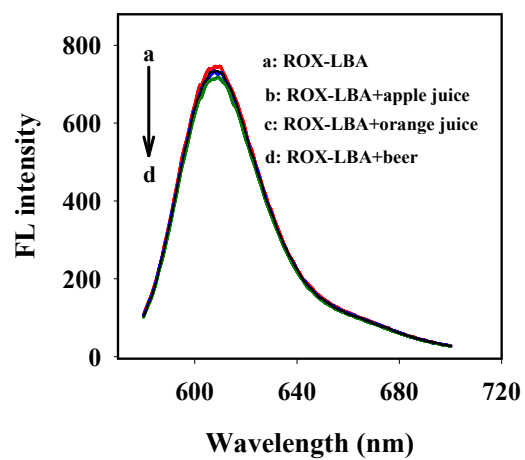
Fig.S3.

Fig.S3. Fluorescence emission spectra of ROX–LBA with different real samples. The real samples were diluted 10 times for analysis.

Table S1

Comparison of different methods for detection of lipopolysaccharide.

Method	Linear range	Detection limit [a]	Reference
Fluorescence detection (Peptide–perylene)	—	280 ng mL^{-1}	17
Colorimetric method (Gold nanorods)	0.01–0.6 μM	8.4 nM (84 ng mL^{-1})	20
Colorimetric detection (peptide and AuNPs)	10–1000 nM	2 nM (20 ng mL^{-1})	22
Surface enhanced Raman scattering sensing	33–667 μg mL^{-1}	21 μg mL^{-1}	23
Electrochemical detection	0.01–1 ng/mL	—	26
Surface plasmon resonance smartphone	50 ng m L^{-1}–180μg/mL	32.5 ng/mL	53
Fluorescence detection (cationic platinum complexes)	—	5.7 nM (57 ng mL^{-1})	54
Fluorescence sensing (gold nanoparticle)	—	0.65 nM (6.5 ng mL^{-1})	55
Colorimetric analysis	10 pg/mL –180μg/mL	0.22 pg/mL	56
Electrochemical detection	0.02–200 ng mL^{-1}	2 ng mL^{-1}	57
Fluorometric sensing (CTAB capped gold)	0.5–50 nM.	0.56 nM (5.6 ng mL^{-1})	58
Fluorescence detection (aptamer-based probe)	25–1600 ng mL^{-1}	15.7 ng mL^{-1}	This work

a: The LPS molecular weight was measured to be 10 kDa in previous work[6]

Molecular docking steps

The structure of lipopolysaccharide was developed through ChemBioDraw Ultra 14.0, which was transferred to 3D structure by using ChemBio3D Ultra 14.0 and further optimized by MMFF94 force field and saved in the form of mo12. Simultaneously, SYBYL-X 2.0 was adopted to develop the 3D structure of lipopolysaccharide aptamer and saved in the form of pdb. After the lipopolysaccharide and aptamer were transferred to PDBQT form through AutodockTools 1.5.6[59, 60], Autodock vina 1.1.2[61] was used to carry out molecular docking analysis for them. During the analysis, the coordinate of aptamer was set as following: center_x = -0.325，center_y = 1.274，center_z = 0.53；size_x = 12，size_y = 32，size_z = 30.

In order to increase the accuracy of calculation, we set the parameter of exhaustiveness to 15. Unless otherwise stated, default values were used for other parameters. Finally, the conformation with highest score was selected for result analysis by means of PyMoL 1.7.6.

2. Molecular docking analysis

In order to analyze the action mode of lipopolysaccharide with its aptamer from the perspective of molecular, we docked lipopolysaccharide to the binding pocket of aptamer, and the affinity result was shown in Table S2, from which, the affinity between the conformation that has highest scores with its aptamer was -7.5 kcal/mol. The result showed that (Fig.2C in manuscript), the fat long chain of lipopolysaccharide could stretch to nucleotide DA-39, DG-40, DA-41, DT-42, DA-46 and DT-47 in aptamer to form stable hydrophobic interaction. Additionally, lipopolysaccharide could form six hydrogen bonding effects including 2.5 Å, 2.1 Å, 2.4 Å, 2.2 Å, 2.6 Å and 2.3 Å with DA-41, DG-43, DT-45 and DA-46 of nucleotide in its aptamer. Due to these interactions, stable compound was formed by lipopolysaccharide with its aptamer.

Table S2.

The affinity of lipopolysaccharide with its aptamer single-chain DNA

mode	Affinity (Kal/mol)	Dist from best mode	
		rmsd l.b.	rmsd u.b.
1	-7.5	0.000	0.000
2	-7.3	3.519	14.904
3	-7.2	3.178	12.582
4	-7.1	1.638	2.902
5	-7.0	3.475	14.976
6	-7.0	3.342	12.736
7	-6.9	3.196	13.544
8	-6.9	3.593	14.861
9	-6.9	3.390	13.110

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