Supplementary Material

A colorimetric aptasensor based on NH_2-MIL-88B for highly selective detection of trace oxytetracycline in water

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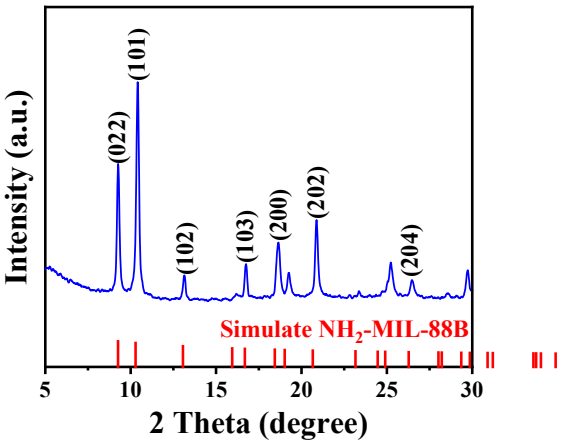

Fig. S1 The XRD pattern of NH_2-MIL-88B.

As shown in Fig. S1, the observed characteristic peaks at 9.26°, 10.40°, 13.14°, 16.75°, 18.65°, 20.88° and 26.47° were corresponded to the (022), (101), (102), (103), (200), (202) and (204) planes of NH_2-MIL-88B respectively, which were consistent with the simulated NH_2-MIL-88B. The results of XRD pattern of NH_2-MIL-88B indicated the successful synthesis of NH_2-MIL-88B.

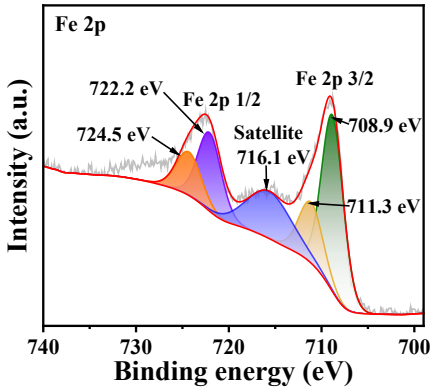

Fig. S2 The high-resolution spectra of Fe 2p for NH_2-MIL-88B.

Fig. S2 exhibited the high-resolution XPS spectra of Fe 2p. Two peaks at 722.5 and 709.1 eV were corresponded to Fe 2p1/2 and Fe 2p3/2 respectively, which could be split into several peaks at 724.5, 722.2, 711.3, and 708.9 eV belonging to Fe^{3+}. Meanwhile, the shaking satellite of Fe^{3+} at 716.1 eV could be observed [1, 2]. The high-resolution XPS spectra of Fe 2p showed that Fe^{3+} species were the main active

sites in the NH_2-MIL-88B, which played an important role in accelerating the redox reaction between H_2O_2 and TMB.

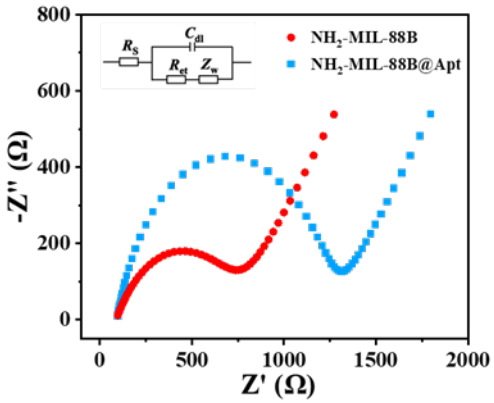

Fig. S3 EIS Nyquist plots of NH_2-MIL-88B and NH_2-MIL-88B@Apt.

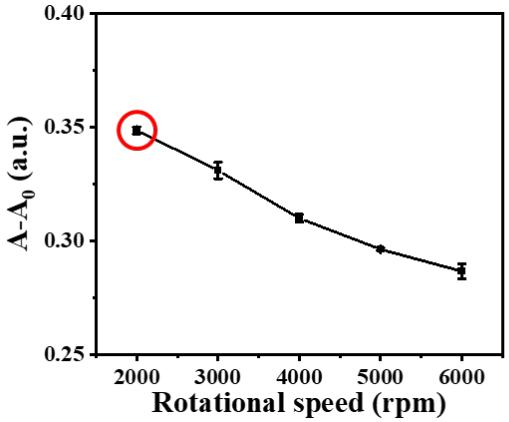

Fig. S4 Effect of centrifugal rotational speed on the colorimetric aptasensor for OTC detection.

Table S1

A comparison of the methods for OTC detection.

Method	Probe type	LOD (M)	Detection range (M)	References
SERS	COF_{HB}/ Au NPs	1.40×10^{-11}	5.00×10^{-11}-2.00×10^{-9}	3
Fluorescence	PicoGreen	1.50×10^{-8}	2.00×10^{-10}-2.00×10^{-9} 2.00×10^{-9}-8.00×10^{-7}	4
Fluorescence	AuAg NCs	32.6×10^{-9}	0-5.00×10^{-5}	5
Colorimetry	G-quadruplex DNAzyme	3.30×10^{-9}	2.00×10^{-7}-1.00×10^{-6}	6
Colorimetry	CeO_2 NPs	10.2×10^{-9}	1.00×10^{-7}-8.00×10^{-7}	7
Colorimetry	Au NCs	3.00×10^{-7}	5.00×10^{-7} -1.50×10^{-5}	8
Colorimetry	NH_2-MIL-88B	1.90×10^{-11}	1.00×10^{-10}-3.00×10^{-7}	This work

Real samples analysis by UPLC-MS/MS

The water samples were filtered through 0.22 μm filter membrane and then directly tested by UPLC-MS/MS.

Chromatographic methods

UPLC was carried out on an Acquity Cortecs UPLC C18 column (1.6 μm particle size, 2.1 mm × 100 mm, Waters) at 40℃. The mobile phase consisted of a 0.1% formic acid-water solution (eluent A) and pure methanol (eluent B). The gradient elution program was as follows: 0 ~ 1 min, 80% A; 0.1 ~ 7.0 min, 20% A; and 7 ~ 8 min, 80% A. The total run time was 8 min, the flow rate was set at 0.35 mL/min, and the injection volume was 5 μL.

MS/MS conditions

The mass spectrometer was operated in positive ion and negative ion modes as well as multiple reaction monitoring mode. The specific parameters are shown below: source

temperature 150°C, desolvation temperature 500°C, capillary voltage + 2.5 / − 0.8 kV, conical gas flow rate 150 L h^{-1}, desolvation gas flow rate 1000 L h^{-1}, capillary voltage 150 L h^{-1}, and conical gas flow rate 150 L h^{-1}.

References

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