Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting information:

A novel molecularly imprinted polymers on metal organic frameworks as sensor for highly selective detection of zearalenone in wheat

Qiuzheng Du[1], Pu Wu[1], Fan Hu[1], Geyuan Li[1], Jianrong Shi[*2 3 4], Hua He[*1 5 6]

1 Department of Analytical Chemistry, China Pharmaceutical University, Nanjing 211198, China

2 Key Laboratory of Food Quality and Safety of Jiangsu Province-State Key Laboratory Breeding Base, Nanjing 210014, China

3 Key Laboratory of Control Technology and Standard for Agro-product Safety and Quality, Ministry of Agriculture, Nanjing 210014, China

4 Key Laboratory of Agro-product Safety Risk Evaluation, Ministry of Agriculture, Nanjing 210097, China

5 Key Laboratory of Biomedical Functional Materials, China Pharmaceutical University, Nanjing 211198, China

6 Key Laboratory of Drug Quality Control and Pharmacovigilance, Ministry of Education, China Pharmaceutical University, Nanjing 210009, China

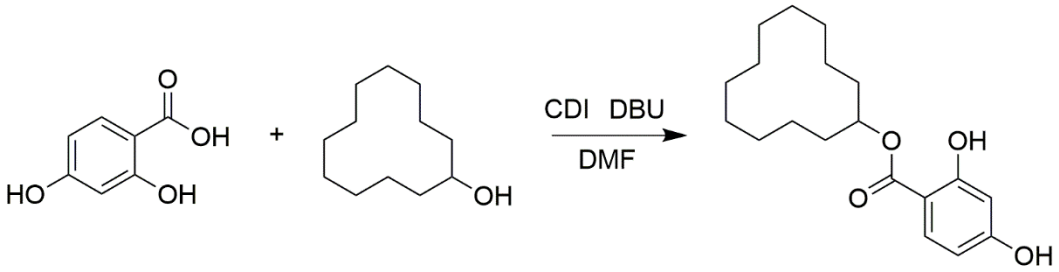
Corresponding Authors

* To whom correspondence should be addressed: China Pharmaceutical University, 639 Longmian Avenue, Nanjing 211198, Jiangsu Province, China. Tel.: +86 025 86185160; E-mail addresses: jcb_321@163.com, dochehua@163.com (H. He) and Institute of Food Safety and Nutrition，Jiangsu Academy of Agriculture Science, Nanjing 210014, China, jianrong63@126.com (J.R. Shi).

Qiuzheng Du and Pu Wu contributed equally to this work and should be considered co-first authors.

From the analysis of CDHB structure, the compound can be obtained by condensation of 2,4-dihydroxybenzoic acid and cyclododecanol. Since the steric hindrance of cyclododecanol is relatively large, direct esterification is difficult. The two phenolic hydroxyl groups on 2,4-dihydroxybenzoic acid are acidic and the nucleophilicity is weaker than that of the fatty alcohol, so it can be made into an active amide or an active ester which is relatively easy to leave. In the presence of fatty alcohols, the reactive intermediate preferentially reacts with the fatty alcohol and the intermediate state activity is moderate, which can reduce the possibility of dimerization or polymerization of 2,4-dihydroxybenzoic acid [1]. Considering that CDI was cheap and could be esterified in one pot, it was made into an active imidazole amide with moderate activity. Due to the mild reaction conditions and simple operation, it was suitable for amplification. The synthetic route map is shown in scheme S1.

To demonstrate CDHB completely be removed, we used UV-Vis spectrometer to detect CDHB in the washing solution. Fig. S1 showed that there were no UV adsorption peaks at 259 and 298 nm in the UV-vis spectrum of the washing solution, which were the characteristic peaks of CDHB. Compared the UV-vis spectra of washing solutions of MMIP and MNIP, it showed that CDHB had been completely removed.



Scheme S1. Schematic representation of CDHB synthesis.

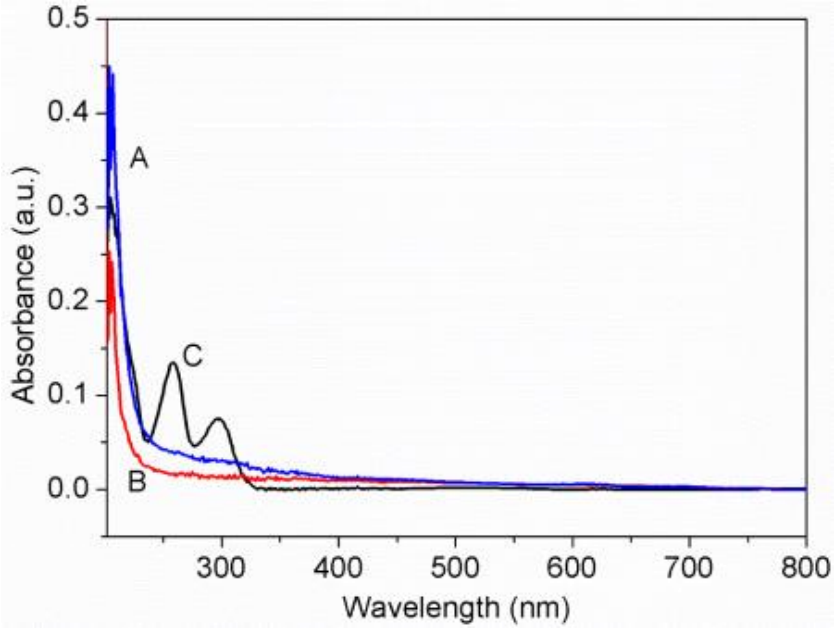


Fig. S1. UV-vis spectra of washed solutions of MMIP (A) and MNIP (B), and UV-vis spectra of CDHB (C).

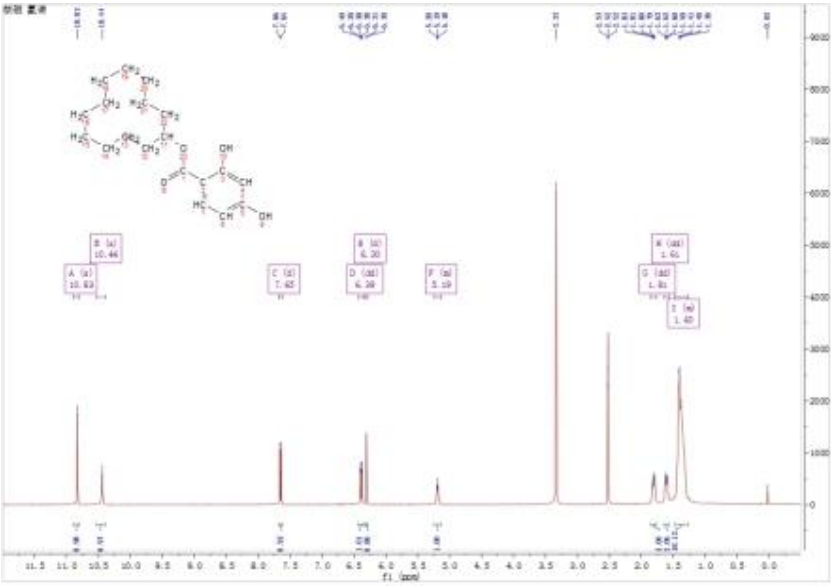


Fig. S2. ^{1}H NMR spectra of CDHB.

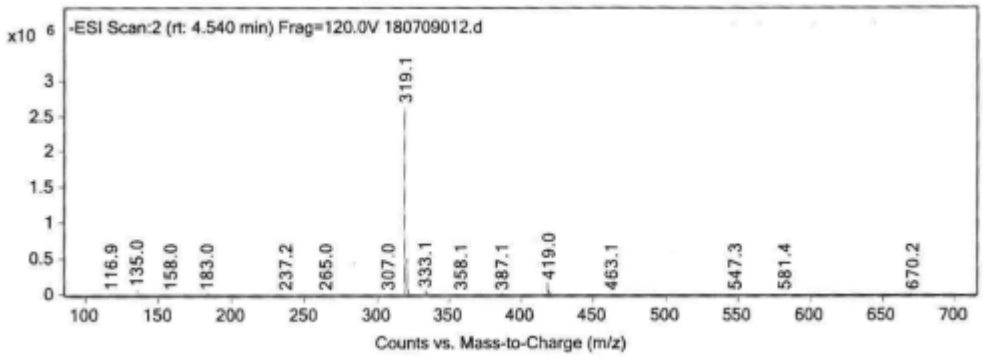


Fig. S3. Negative ion mass spectra of CDHB.

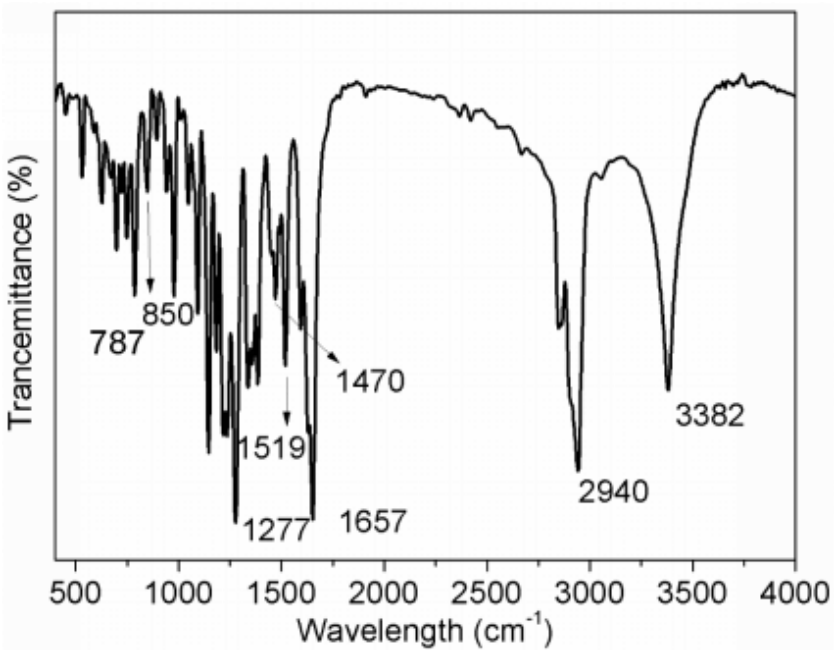


Fig. S4. FT-IR spectra of CDHB.

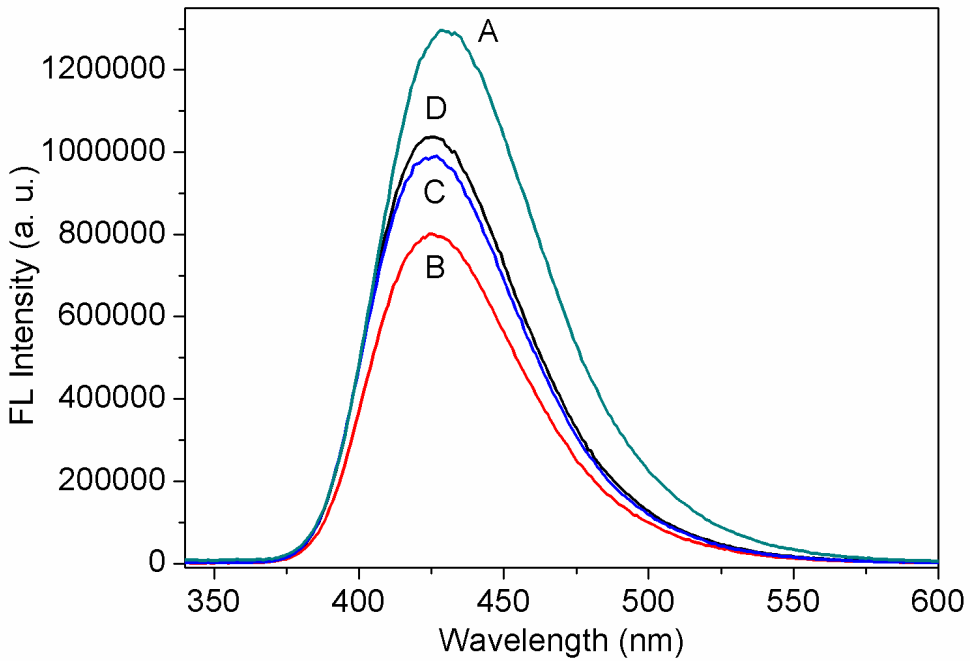


Fig. S5. Fluorescence spectra of MOF (A), MMIP before (B) and after (C) template extraction, MNIP (D).

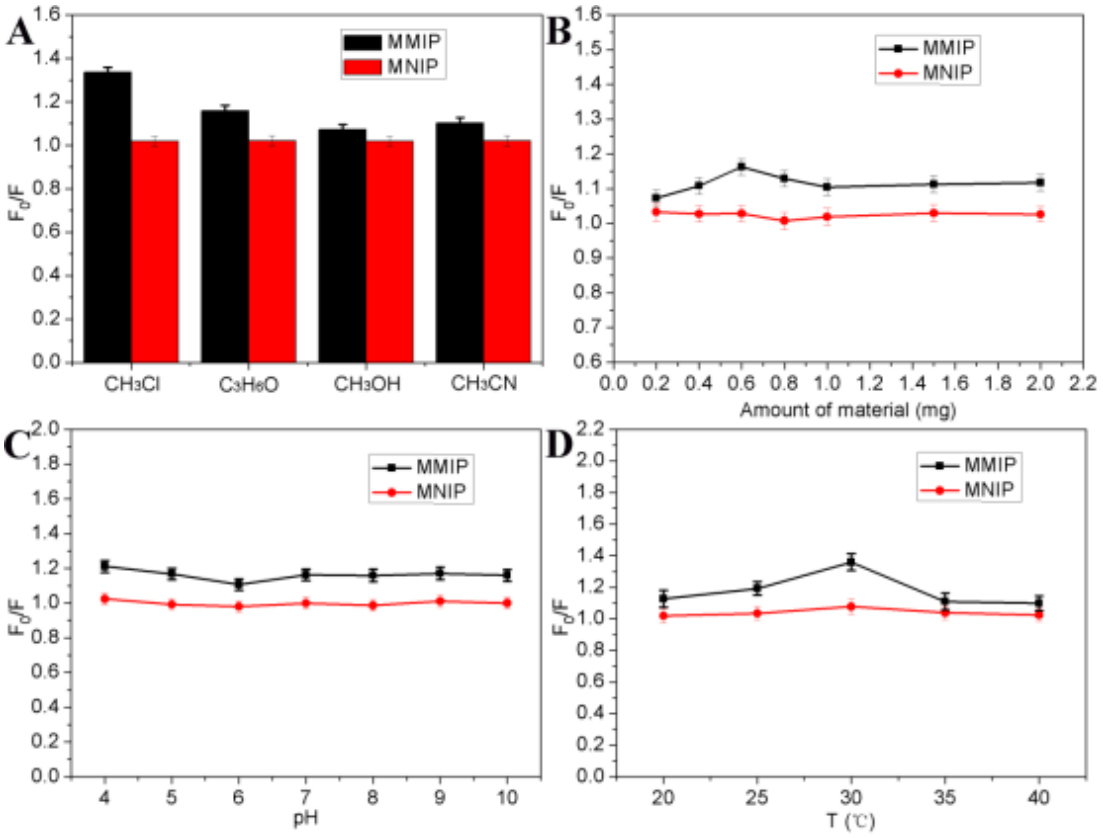


Fig. S6. Optimization of optimal adsorption conditions: adsorption medium (A), material amount (B), pH value (C) and adsorption temperature (D).

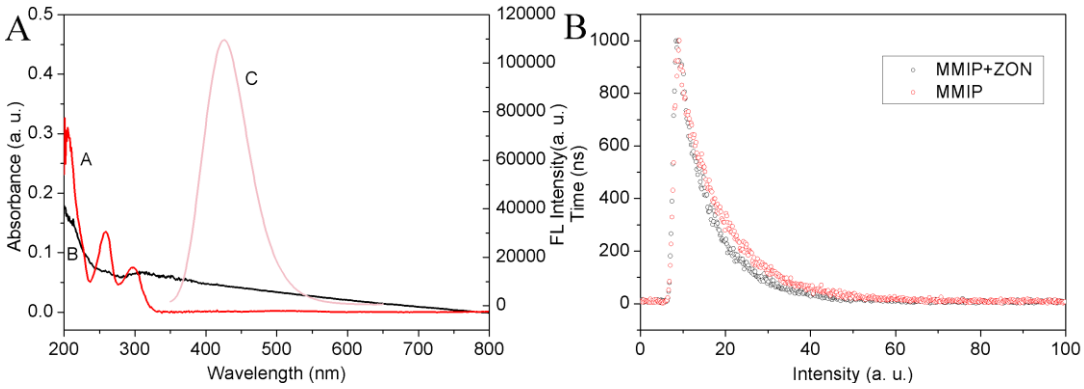


Fig. S7. (A) UV-vis spectra of ZON standard solution (A) and MMIP (B), fluorescence emission spectra of MMIP (C); (B) Fluorescence lifetime of MMIP and a mixture of MMIP and ZON.

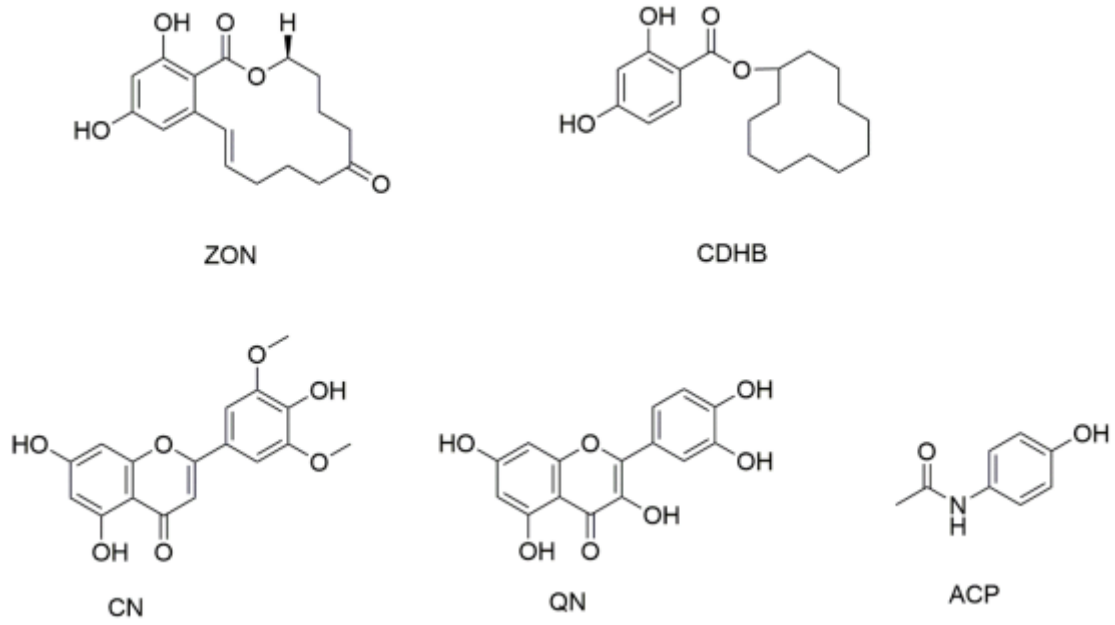


Fig. S8. Structure of ZON, CDHB, CN, QN and ACP.

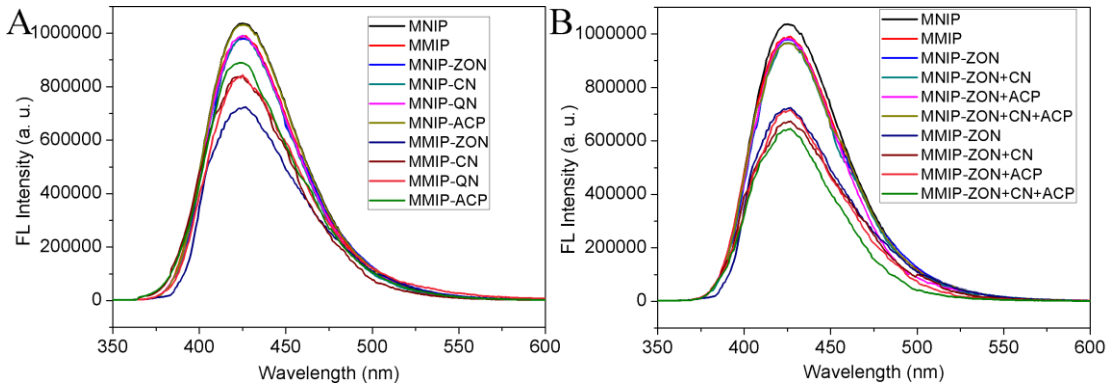


Fig. S9. Fluorescence spectra of selective adsorption (A) and competitive adsorption (B) of MMIP and MNIP.

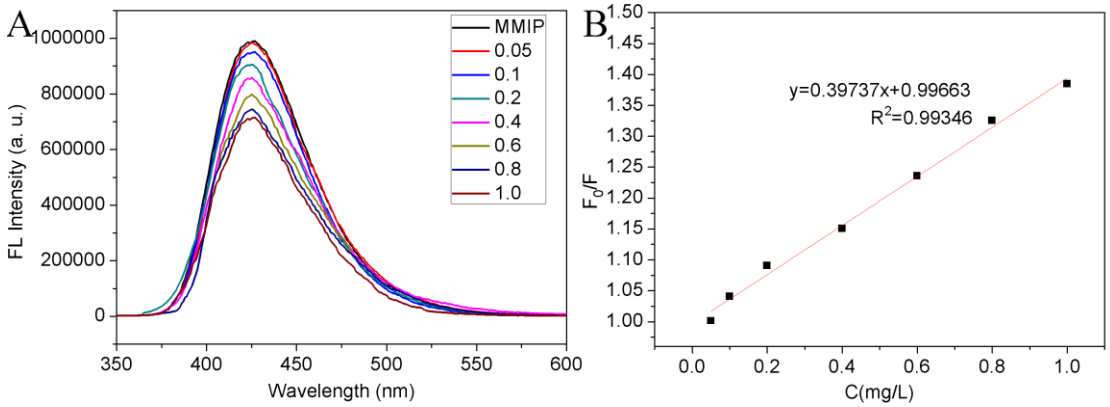


Fig. S10. (A) Fluorescence spectra of MMIP at different concentrations of ZON, (B) standard curve line of fluorescent sensor.

Reference

1. J. L. Urraca, M. D. Marazuela, E. R. Merino, G. Orellana and M. C. Moreno-Bondi, *Journal of chromatography. A*, 2006, **1116**, 127-134.