# A stable Zn-coordination polymer for the quantitative and selective detection of biomarker phenylglyoxylic acid in urine

Rongqi Wang[2,3,†], Ruxue Wang[4,†], Zeqin Chen[1], Laiwen Li[1], Xinyu Zong[5], Jing Wang[1,*], Ziao Zong[1,*]

[1]Key Laboratory of Research on Environmental Pollution and Health Risk Assessment, Youjiang Medical University for Nationalities, Baise, Guangxi 533000, PR China

[2]Affiliated Hospital of Youjiang Medical University for Nationalities, Baise, Guangxi 533000, China

[3]Key Laboratory of Biomedical Material Research of Guangxi (Cultivation), Baise, Guangxi 533000, China

[4]College of Biological Engineering, Qingdao University of Science and Technology, Qingdao, Shandong 266042, P.R. China

[5] School of Public Health, Guilin Medical University, Guilin, Guangxi 541199, P.R. China

*Correspondence: wangjing@ymcn.edu.cn (J. W) zongziao@126.com (Z.-A. Z)

† These authors contributed equally to this work.

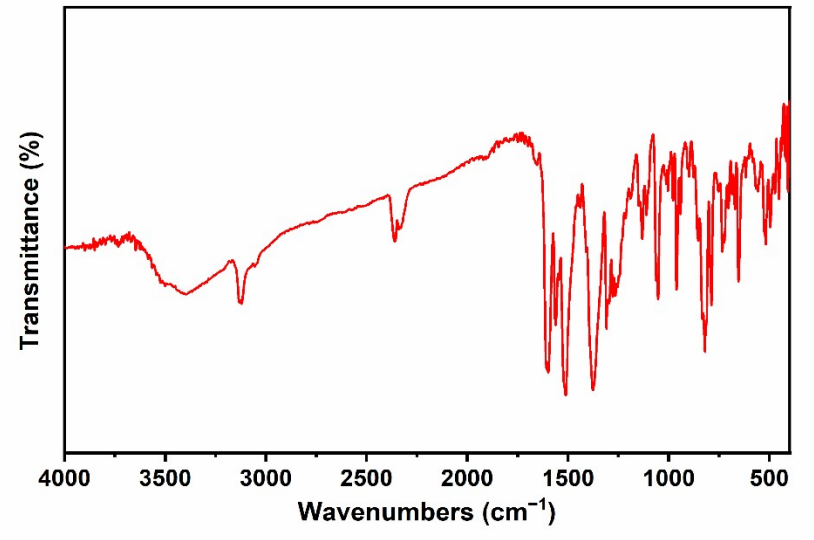


Figure S1 FT-IR curves of **1**.

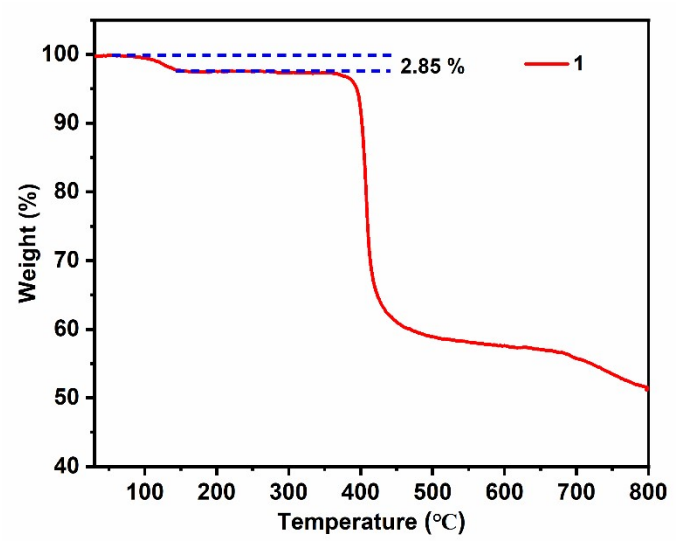


Figure S2 TGA curves of **1**.

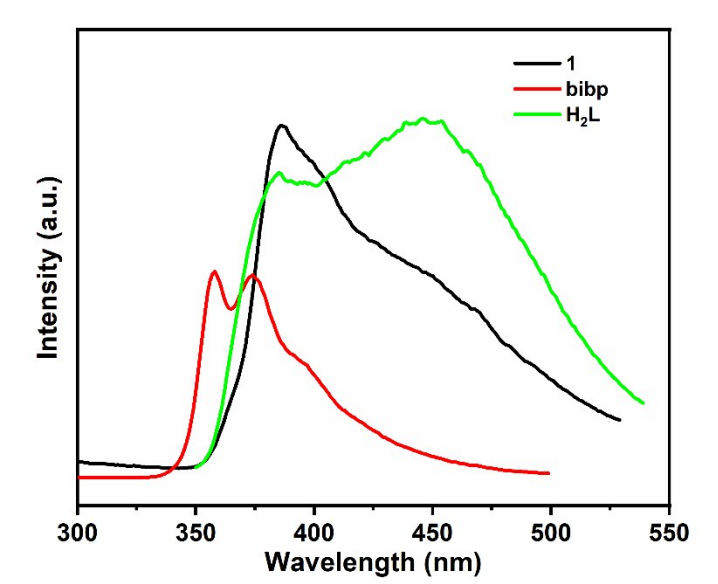


Figure S3 Solid-state fluorescence emissions of **1**, $H_2L$ and bibp.

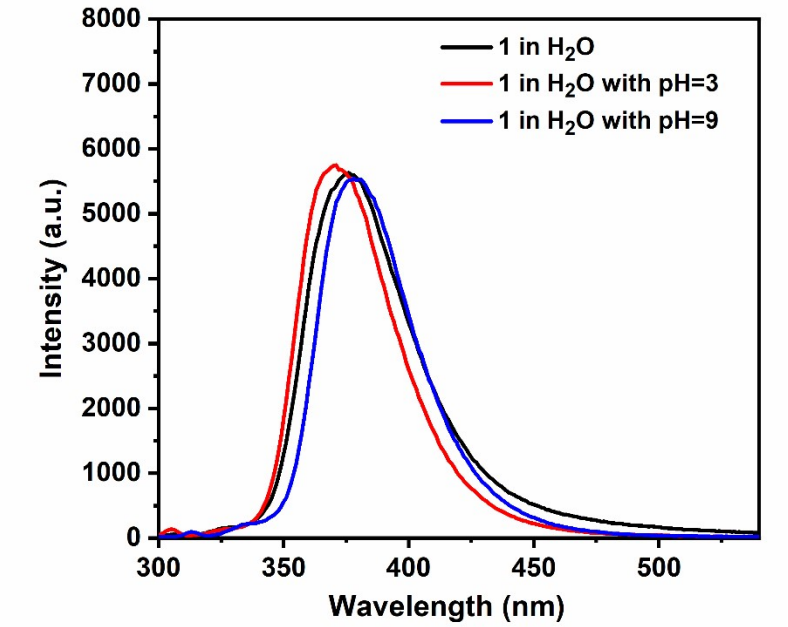


Figure S4 Fluorescence emissions of **1** in aqueous solutions with different pH values.

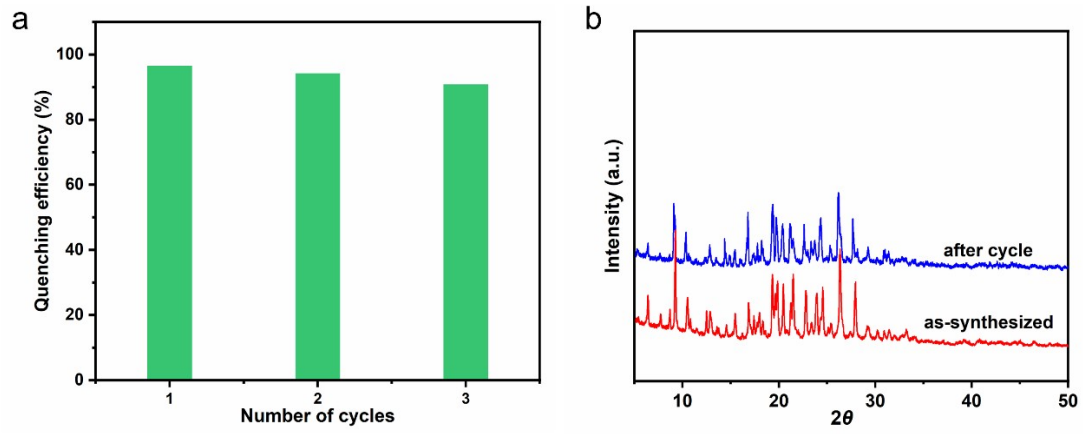


Figure S5 (a)Cyclic stability of **1** for the detection of PGA. (b) PXRD patterns of **1** before and after soaking in the solution of PGA.

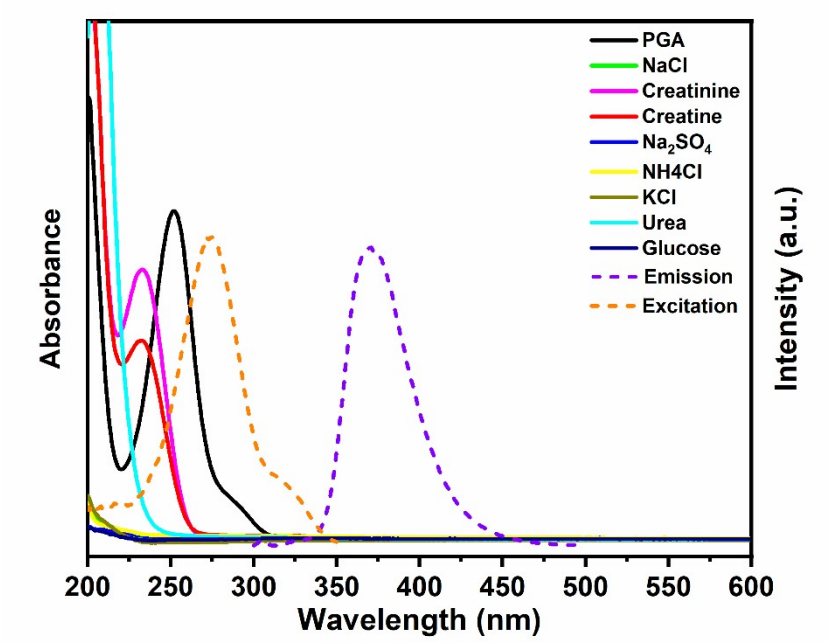


Figure S6 UV–Vis absorption spectra of different urine components and the fluorescence emission/excitation bands of **1** in water.

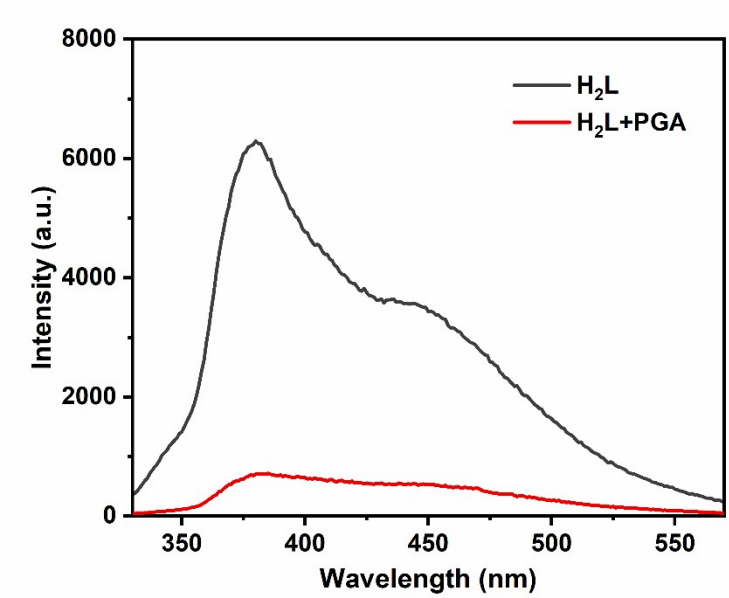


Figure S7 The behaviour with $H_2L$ alone to detect PGA.

Table S1 Selected bond lengths (Å) and angles (°) for **1**

| Selected bond lengths | | Selected bond lengths angle | |
|---|---|---|---|
| Zn1—O2 | 1.955(2) | O2—Zn1—O3$^{i}$ | 108.67(10) |
| Zn1—O3$^{i}$ | 1.959(2) | O2—Zn1—N1 | 121.58(11) |
| Zn1—N1 | 2.008(3) | O2—Zn1—N4$^{ii}$ | 109.40(11) |
| Zn1—N4$^{ii}$ | 2.036(3) | O3$^{i}$—Zn1—N1 | 112.45(11) |
| | | O3$^{i}$—Zn1—N4$^{ii}$ | 95.92(11) |
| | | N1—Zn1—N4$^{ii}$ | 105.67(11) |

Symmetry code: (i) *x*-1/2, -*y*+1/2, *z*+1/2; (ii) -*x*+7/2, *y*+1/2, -*z*+3/2.

Table S2 Non-bonding interactions geometry (Å, °)

| Complex | D—H…A | d(D—H) | d(H…A) | d(D…A) | ∠DHA |
|---|---|---|---|---|---|
| **1** | $O_5$—$H_{5A}$…$N_9$ | 0.767 | 2.286 | 2.937 | 143.27 |
| | $C_{20}$—$H_{20}$…$O_5$ | 0.940 | 2.364 | 3.116 | 136.78 |
| | $C_{62}$—$H_{62}$…$O_1$ | 0.940 | 2.612 | 3.205 | 121.55 |
| | $C_{14}$—$H_{14}$…$O_5$ | 0.940 | 2.691 | 3.605 | 164.35 |

Table S3 Comparison of various methods used for sensing PGA

| Method | Material | Sample | LOD (μM) | Ref |
|---|---|---|---|---|
| Luminescence | LCP 1 | Water | 3.4 | S1 |
| | LCP 2 | Water | 3.8 | |
| | LCP 3 | Water | 5.8 | |
| HPLC-MS | / | Urine | 6.67 | S2 |
| Capillary electrophoresis (CE) | / | Urine | 20 | S3 |
| Voltammetry | / | Urine | 33 | S4 |
| Potentiometry | Salen-Co(III) | Water | 1.96 | S5 |
| Luminescence | **1** | Urine | 2.67 | This work |

Table S4 **1** was used to detect the concentration of PGA in human urine.

| Complex | Add (μM) | Found (μM) | Recovery (%) | RSD (%) |
|---|---|---|---|---|
| **1** | 5.00 | 4.73 | 94.60 | 3.57 |
| | 10.00 | 11.54 | 115.40 | 3.48 |
| | 15.00 | 14.92 | 99.47% | 2.31 |

## References


[S1] S. Wu , M. Zhu , Y. Zhang , M. Kosinova , V. P. Fedin and E. Gao , Appl. Organomet. Chem., 2020, 35.

[S2] J. Z. Wang , X. J. Wang , Y. H. Tang , S. J. Shen , Y. X. Jin and S. Zeng , J. Chromatogr. B: Anal. Technol. Biomed. Life Sci., 2006, 840, 50—55.

[S3] C. Y. Wang , C. T. Huang and Y. Z. Hsieh , J. Sep. Sci., 2003, 26, 69—74.

[S4] T. Navrátil , Z. Šenholdová , K. Shanmugam and J. Barek , Electroanalysis, 2006, 18 , 201—206.

[S5] B. Li , J. Hou , Y. Y. ang , S. Chen and L. Xu , Chem. Sens., 2011, 01.