

Electronic Supplementary Information (ESI)

Stable bifunctional Zn^{II}-based sensor toward acetylacetone and L-histidine by a fluorescence red shift and turn-on effect

Shu-Li Yao, Hui Xu, Teng-Fei Zheng, Yan Peng, Sui-Jun Liu,* Jing-Lin Chen and He-Rui Wen*

School of Chemistry and Chemical Engineering, Jiangxi Provincial Key Laboratory of Functional Molecular Materials Chemistry, Jiangxi University of Science and Technology, Ganzhou 341000, Jiangxi Province, P.R. China

*Corresponding authors. E-mail: sjliu@jxust.edu.cn (S.-J. Liu), wenherui63@163.com (H.-R. Wen). Tel: +86-797-8312204, +86-797-8312289.

Table S1. Selected bond lengths (Å) and angles (°) for **JXUST-15**.^a

Zn1—O1	1.958(13)	Zn1—N1 ⁱ	2.0280(17)
Zn1—N1	2.0280(17)	Zn1—O1 ⁱ	1.958(13)
O1—Zn1—N1	113.9(4)	N1—Zn1—N1 ⁱ	95.86(10)
O1—Zn1—N1 ⁱ	114.9(3)		

^aSymmetry code: (i) $-x+1/2, y, -z+1/2$.

Table S2. SHAPE analysis of Zn^{II} ion in **JXUST-15**.

ion	label	shape	symmetry	distortion(τ)
Zn1	SP-4	Square	D_{4h}	25.798
	T-4	Tetrahedron	T_d	1.919
	SS-4	Seesaw	C_{2v}	6.576
	vTBPY-	Vacant trigonal bipyramid	C_{3v}	4.412

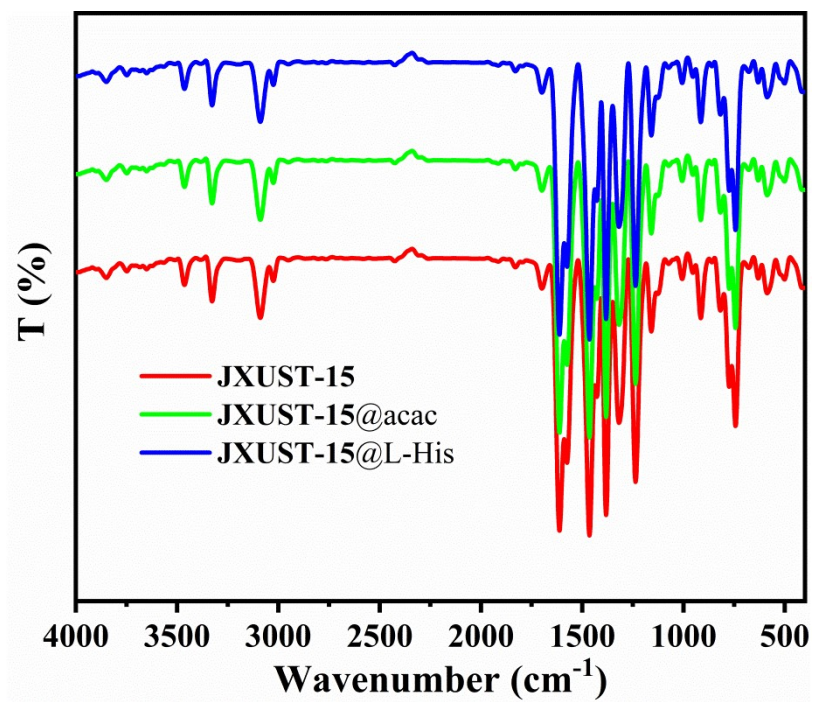


Fig. S1. IR spectra of JXUST-15, JXUST-15@acac and JXUST-15@L-His at room temperature.

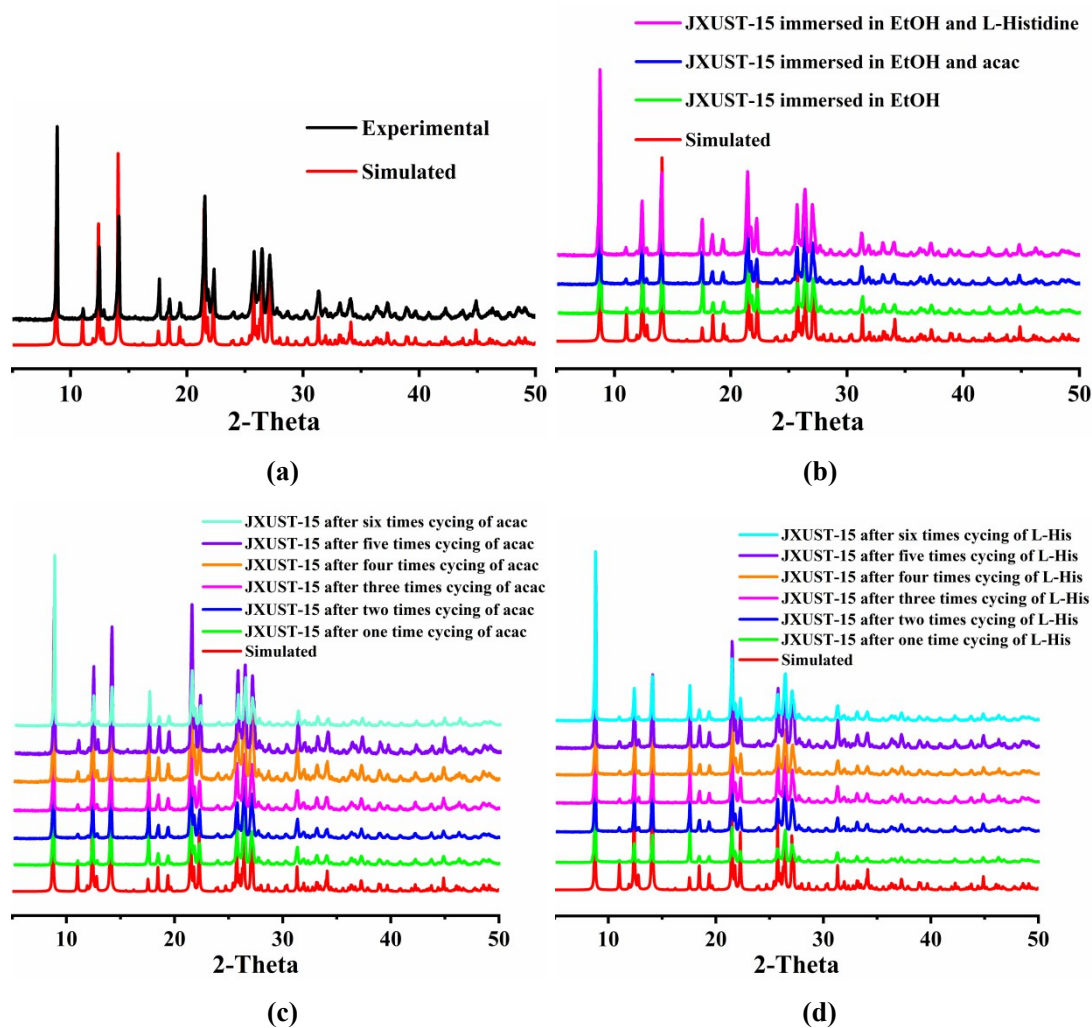


Fig. S2. (a) The simulated and as-synthesized PXRD patterns of **JXUST-15**; (b) PXRD patterns of samples immersed in EtOH, EtOH with acac or L-His solution for 24 h of **JXUST-15**; (c) PXRD patterns of **JXUST-15** after recycling six times of acac with EtOH solution; (d) PXRD patterns of **JXUST-15** after recycling six times of L-His with EtOH solution.

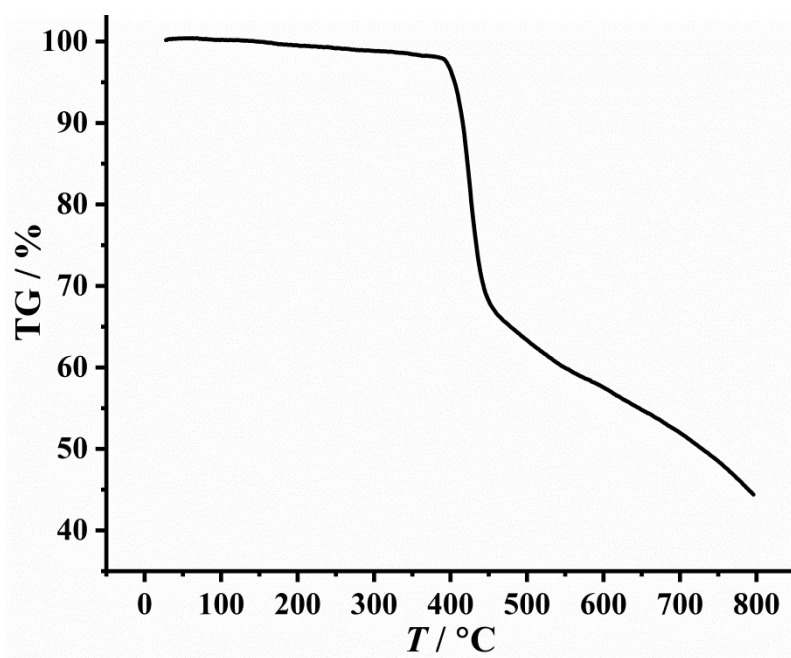


Fig. S3. The TGA curve of **JXUST-15** under N₂ atmosphere from room temperature to 800 °C.

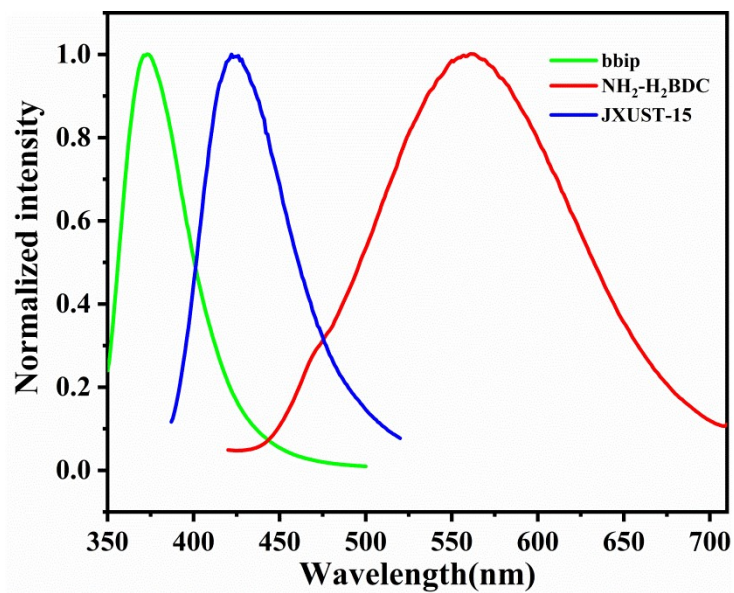
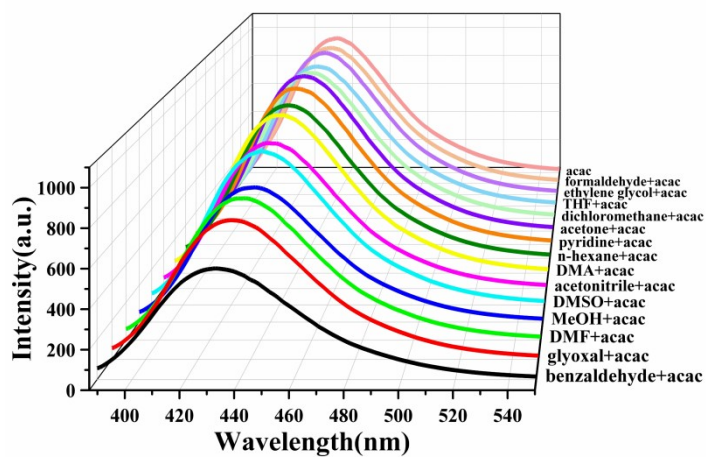
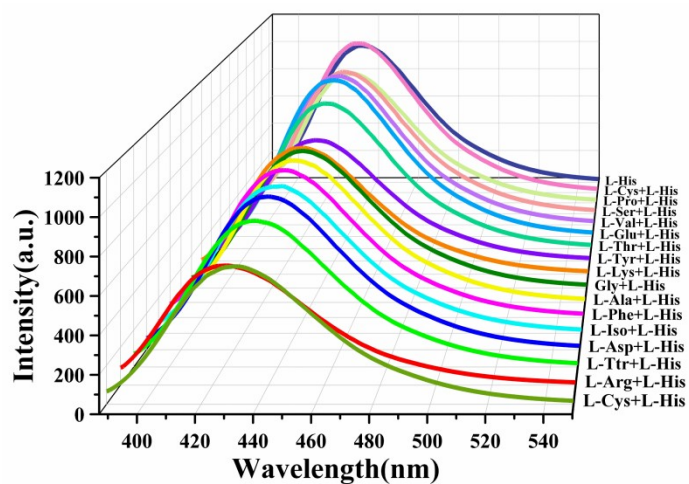


Fig. S4. The solid emission spectra of bbip, NH₂-H₂BDC and JXUST-15.

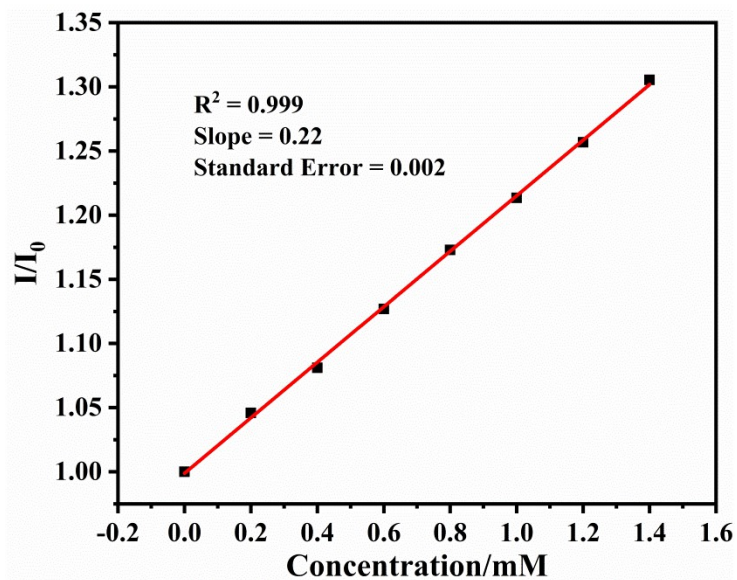


(a)

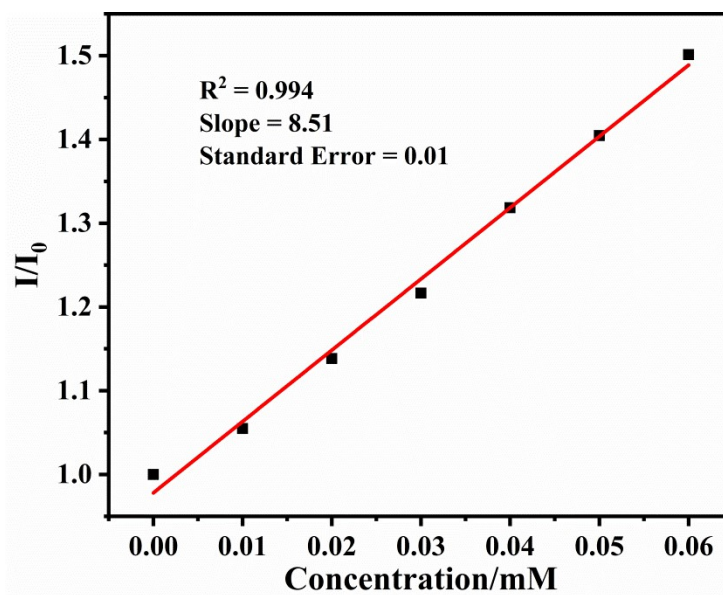


(b)

Fig. S5. The fluorescence response of JXUST-15 dispersed in EtOH suspension with acac and other organic molecules (a) and with L-His and other amino acids (b).

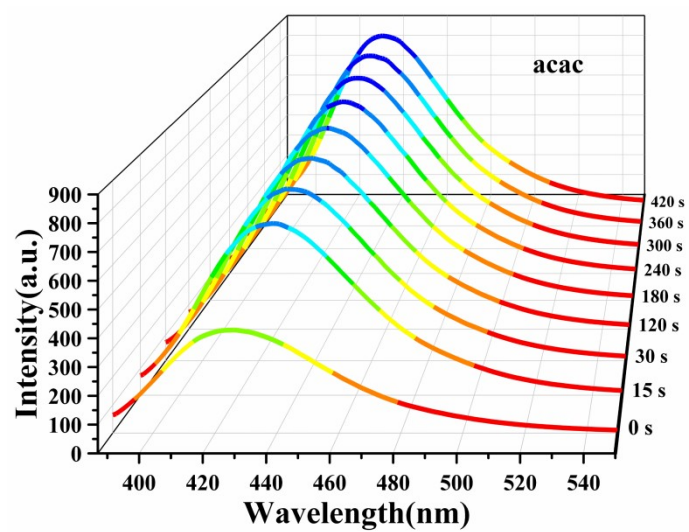


(a)

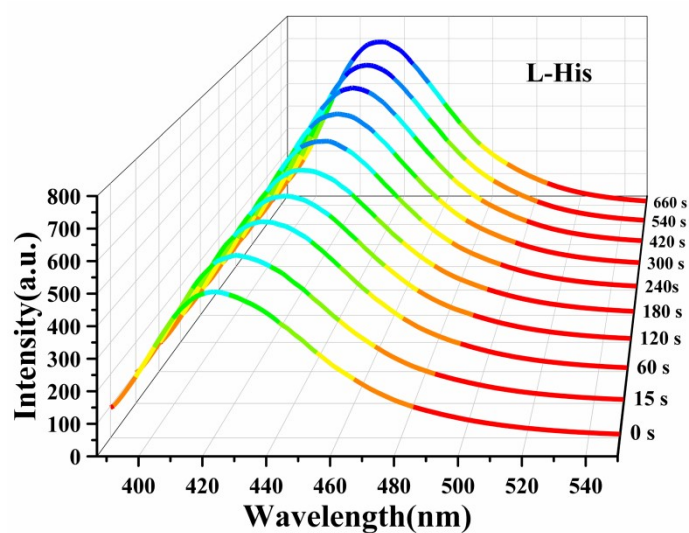


(b)

Fig. S6. The correlation between fluorescence intensity ratio I/I_0 and the concentration of acac (a) and L-His (b) of JXUST-15.

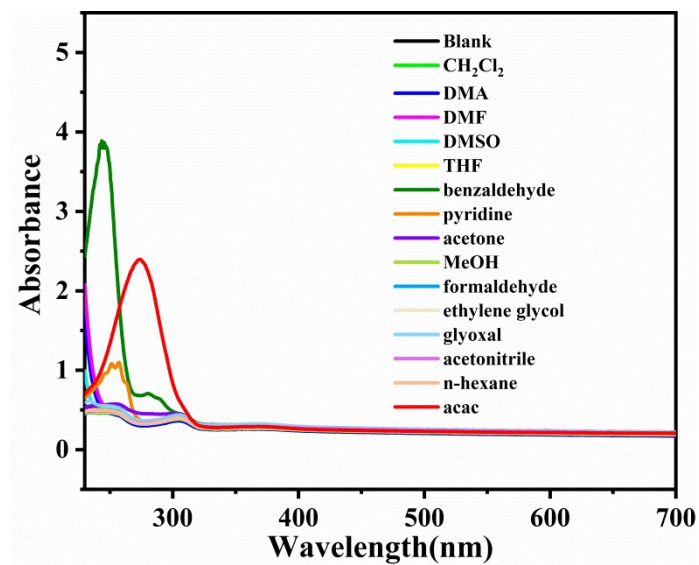


(a)

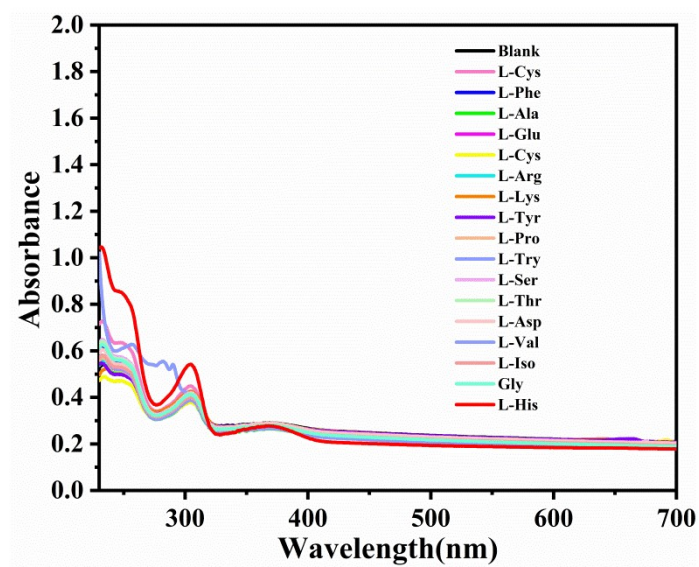


(b)

Fig. S7. Time-dependent fluorescence emission spectra of **JXUST-15** in EtOH suspension with 5 μL acac (a) and 5 μL L-His with the concentration of 0.1 M (b) ($\lambda_{\text{ex}} = 367 \text{ nm}$).

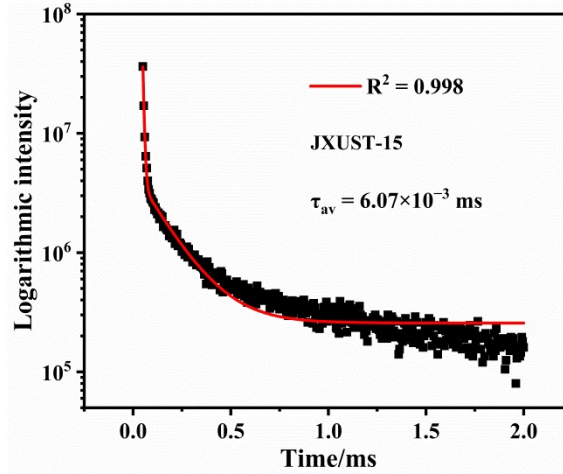


(a)

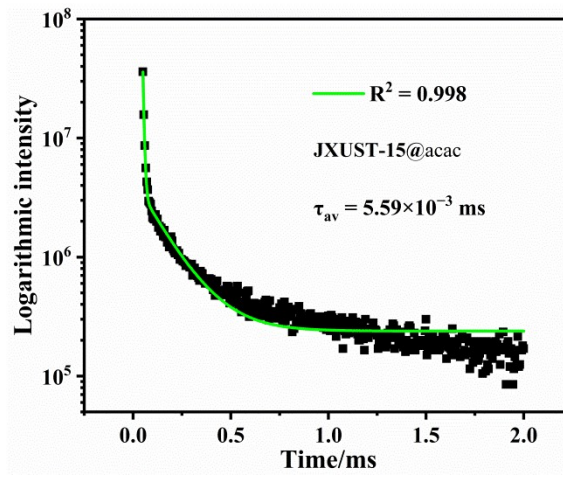


(b)

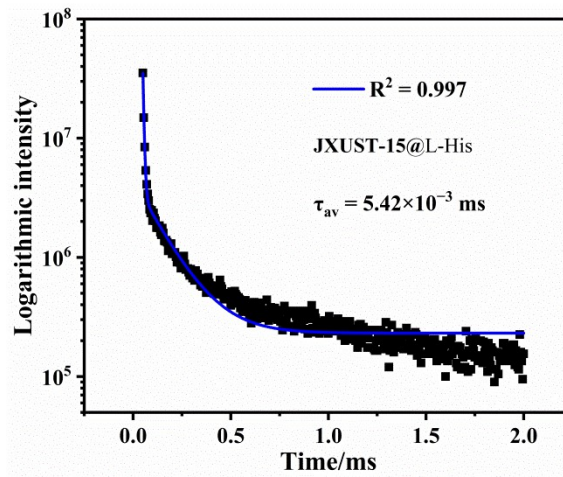
Fig. S8. The UV-Vis absorption spectra of **JXUST-15** and **JXUST-15** upon the addition of (a) different organic molecules and (b) amino-acid solutions.



(a)



(b)



(c)

Fig. S9. The luminescence decay curves of (a) **JXUST-15**, (b) **JXUST-15@acac** and (c) **JXUST-15@L-His** at room temperature ($\lambda_{\text{ex}} = 367 \text{ nm}$ and $\lambda_{\text{em}} = 425 \text{ nm}$).