Electronic Supplementary Information (ESI)

A highly stable and efficient benzothiadiazole-based fluorescence sensor for salicylaldehyde in aqueous solution

Xiao-Long Yan,[a] Xiao-Qin Cao,[a] Cheng-Rui Deng,[a] Teng-Fei Zheng,[a]* Shu-Li Yao[b]* and Sui-Jun Liu[a]*

[a]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

[b]School of Rare Earth and New Materials Engineering, Ganzhou Key Laboratory of Advanced Processing and Technology Optimization of High Performance Tungsten Base Materials, Gannan University of Science and Technology, Ganzhou 341000, Jiangxi Province, P.R. China

E-mail: sjliu@jxust.edu.cn (S.-J. Liu), slyao_gnust@163.com (S.-L. Yao), zhengtengfei0628@163.com. Tel: +86-797-8312204.

Table S1. Selected bond lengths (Å) and angles (°) for **JXUST-27**.

Cd1—N1	2.243(2)	Cd1—N6^{i}	2.2792(19)
Cd1—O4^{ii}	2.3043(18)	Cd1—O1	2.351(2)
Cd1—O2	2.3851(18)	Cd1—O3^{ii}	2.4169(18)
N1—Cd1—O4^{ii}	135.85(7)	O1—Cd1—O2	55.29(6)
N1—Cd1—O1	104.89(7)	N6^{i}—Cd1—O3^{ii}	85.83(7)
O4^{ii}—Cd1—O1	115.01(7)	O1—Cd1—O3^{ii}	165.17(7)
N6^{i}—Cd1—O2	140.82(7)	O4^{ii}—Cd1—O2	98.92(7)
N6^{i}—Cd1—O4^{ii}	104.44(7)	N1—Cd1—O3^{ii}	88.36(7)
N6^{i}—Cd1—O1	86.18(7)	O4^{ii}—Cd1—O3^{ii}	55.39(6)
N1—Cd1—N6^{i}	96.01(7)	O2—Cd1—O3^{ii}	133.29(7)
N1—Cd1—O2	88.33(7)		

Symmetry codes: (i) x, $-y+1/2$, $z-1/2$; (ii) $-x+1$, $y-1/2$, $-z+1/2$.

Table S2. SHAPE analysis of the Cd^{II} ion in **JXUST-27**.

ion	label	shape	symme	distortio
Cd1	HP-6	Hexagon	D_{6h}	29.133
	PPY-6	Pentagonal pyramid	C_{5v}	11.898
	OC-6	Octahedron	O_h	11.585
	TPR-6	Trigonal prism	D_{3h}	**8.412**
	JPPY-6	Johnson pentagonal pyramid J2	C_{5v}	15.455

Table S3. HOMO and LUMO energies for BIBT and SA.

	LUMO	**HOMO**	**Ref.**
SA	-1.78 eV	-6.65 eV	S1
BIBT	-3.07 eV	-6.06 eV	S2

References

S1 K. Wang, T. F. Zheng, J. L. Chen, H. R. Wen, S. J. Liu and T. L. Hu. *Inorg. Chem.*, 2022, **61**, 16177-16184.

S2 J, J. Wang, L. Q. Li, Z. H. Zhu, T. F. Zheng, H. Xu, Y. Peng, J. L. Chen, S. J. Liu and H. R. Wen, *New J. Chem.*, 2022, **46**, 20623-20628.

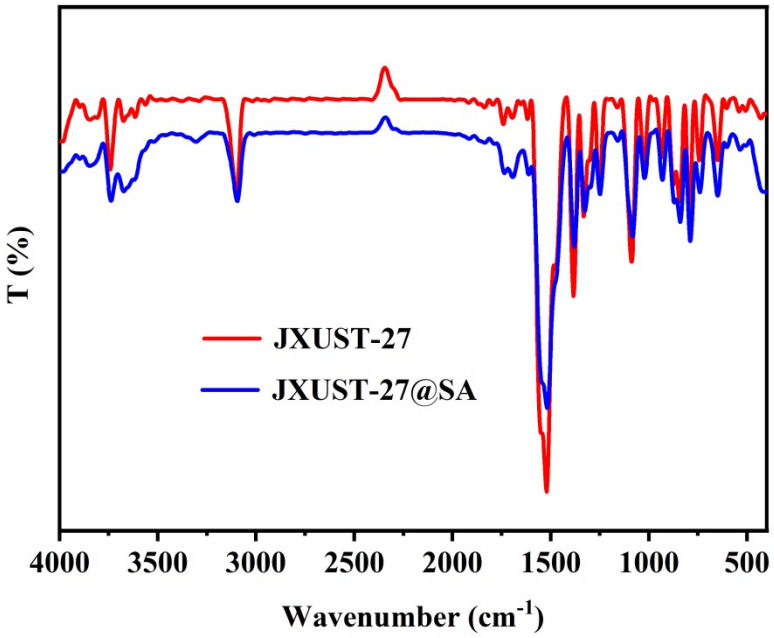


Fig. S1 IR spectra of **JXUST-27** and **JXUST-27**@SA at room temperature.

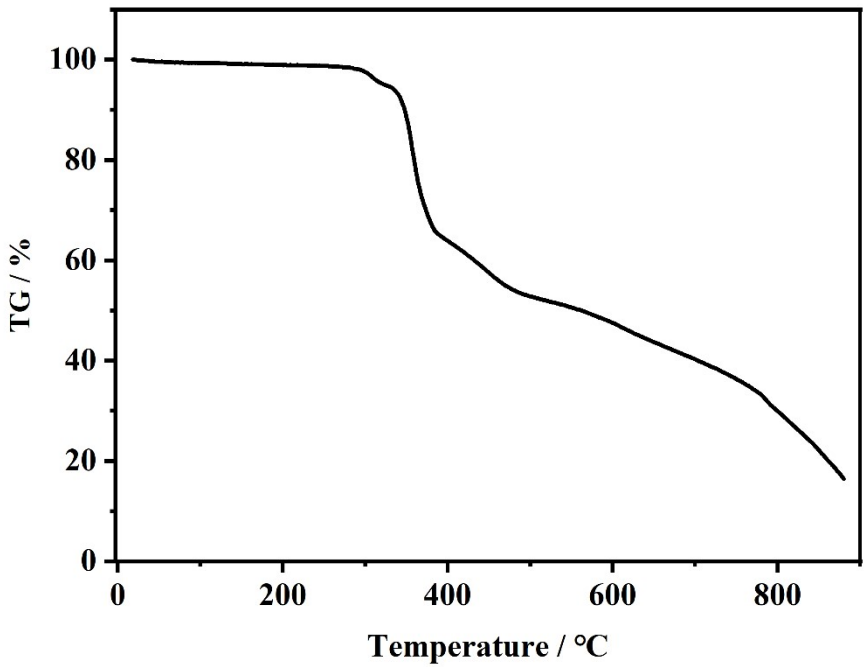
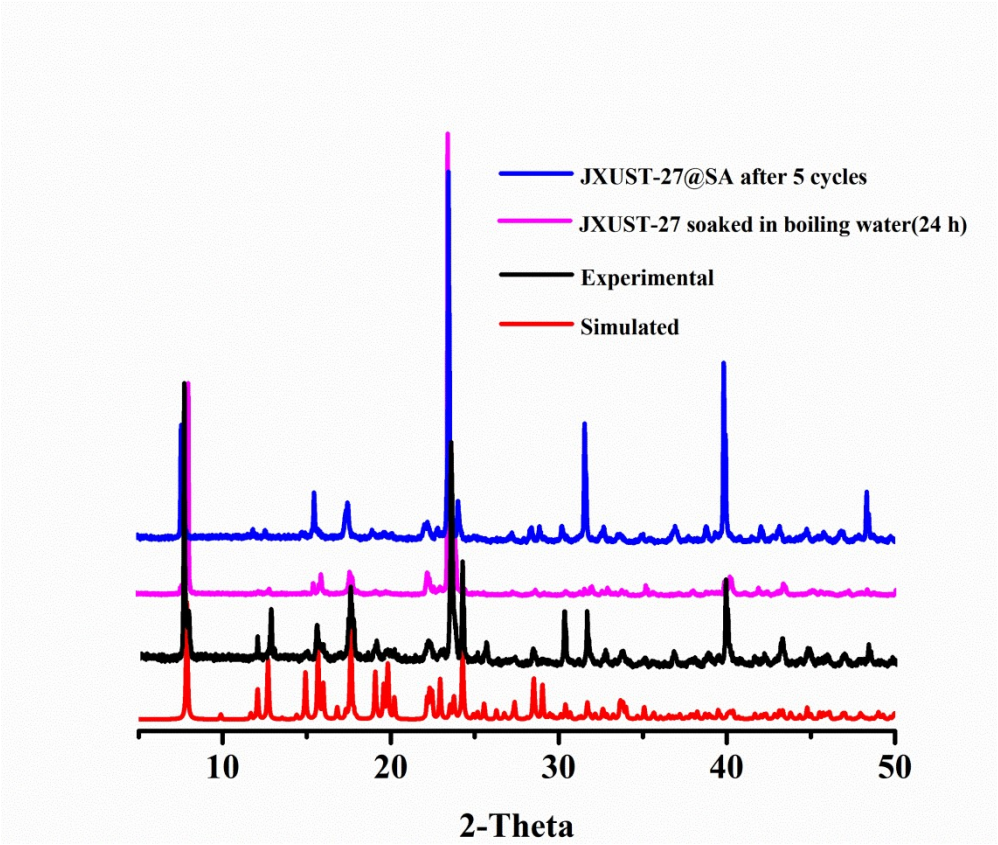
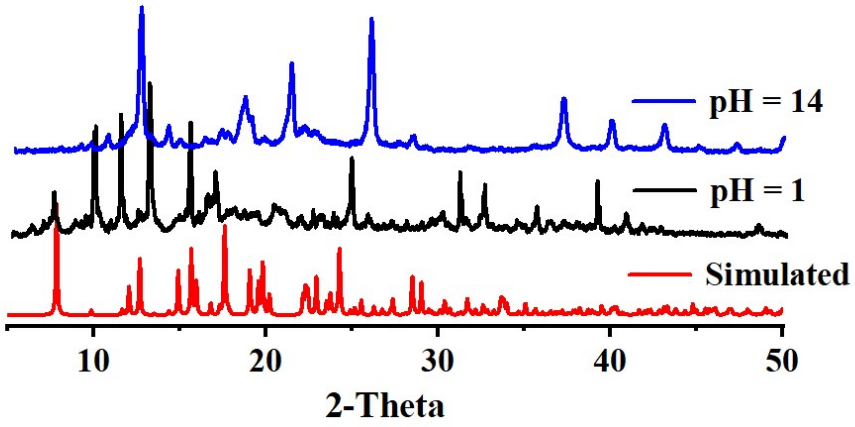


Fig. S2 The TGA curve of **JXUST-27** under N_2 atmosphere.

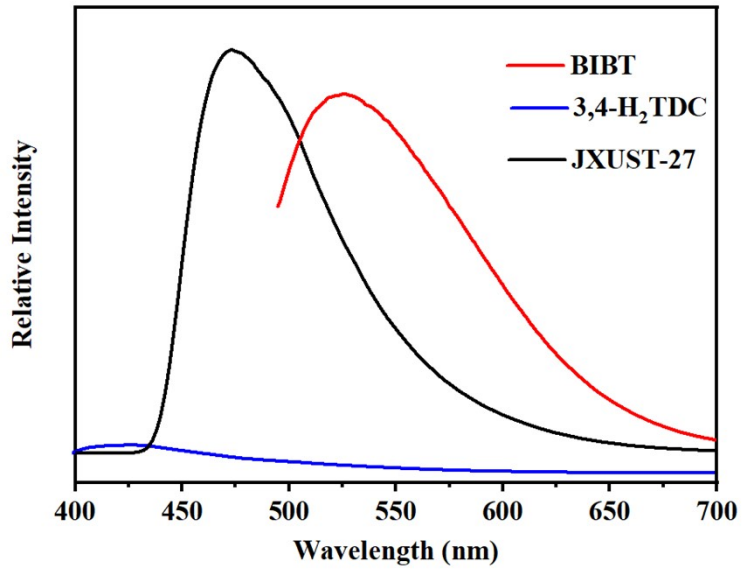


(a)

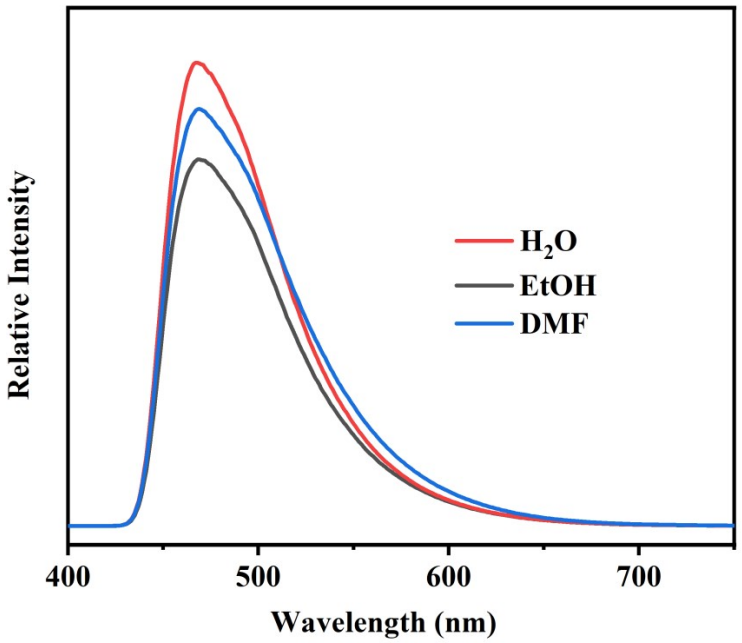


(b)

Fig. S3 (a) The PXRD patterns of as-synthesized **JXUST-27**, **JXUST-27**@SA after 5 cycles and **JXUST-27** after soaked in boiling water for 24 h and the simulated one; (b) the simulated and experimental PXRD patterns of **JXUST-27** immersed in the distinct aqueous solutions with pH values of 1 and 14 for 12 hours.



(a)



(b)

Fig. S4 (a) The solid emission spectra of BIBT, 3,4-H_2TDC and **JXUST-27**; (b) the emission spectra of **JXUST-27** in aqueous, DMF and EtOH solutions.

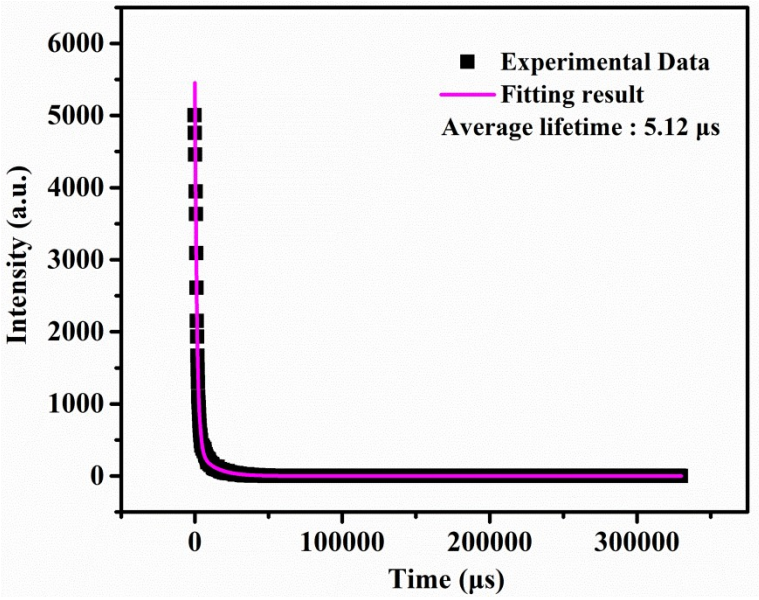


Fig. S5 The luminescence decay curve of **JXUST-27**.

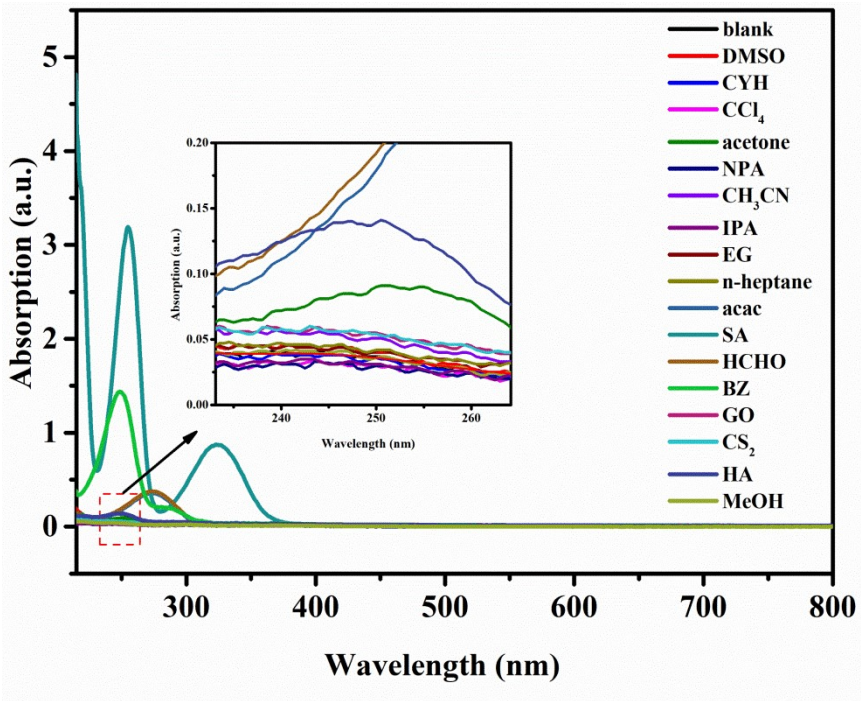


Fig. S6 The UV-Vis absorption spectra of **JXUST-27** and **JXUST-27** upon the addition of different organic molecules.

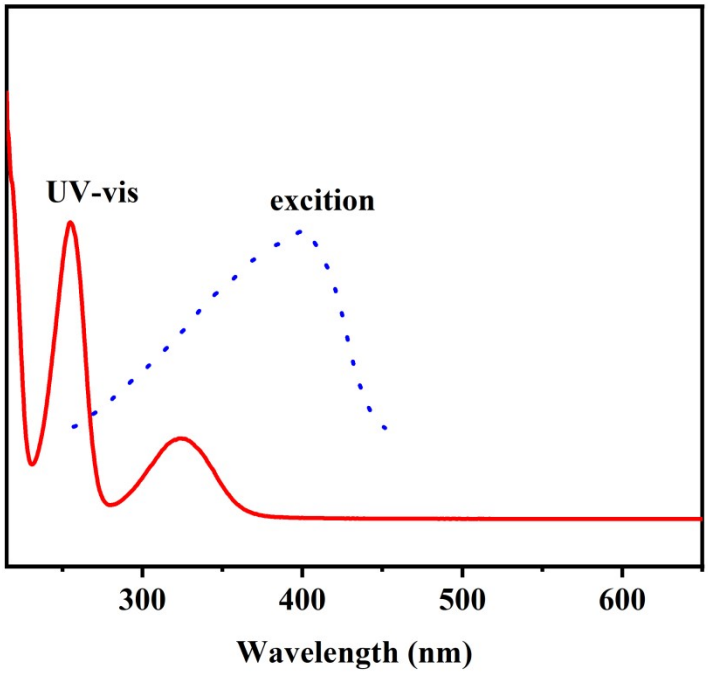


Fig. S7 The UV-Vis absorption spectrum of **JXUST-27**@SA and excitation spectrum of **JXUST-27**.