Electronic Supplementary Information (ESI)

Multifunctional benzothiadiazole-based fluorescence sensor toward Al^{3+}, Cr^{3+} and Fe^{3+}

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Table S1. Selected bond lengths (Å) and angles (°) for **JXUST-3**[a]

Zn1—N1	2.0552(19)	Zn1—O4^{ii}	2.125(3)
Zn1—N6^{i}	2.0699(19)	Zn1—O5^{ii}	2.309(3)
Zn1—O2	2.117(2)	Zn1—O1	2.313(2)
N1—Zn1—N6^{i}	100.37(8)	O2—Zn1—O5^{ii}	103.88(8)
N1—Zn1—O2	99.01(8)	O4^{ii}—Zn1—O5^{ii}	58.70(10)
N6^{i}—Zn1—O2	95.31(8)	N1—Zn1—O1	89.78(8)
N1—Zn1—O4^{ii}	96.22(9)	N6^{i}—Zn1—O1	153.64(8)
N6^{i}—Zn1—O4^{ii}	99.12(9)	O2—Zn1—O1	58.87(8)
O2—Zn1—O4^{ii}	156.75(10)	O4^{ii}—Zn1—O1	103.92(9)
N1—Zn1—O5^{ii}	154.65(9)	O5^{ii}—Zn1—O1	92.77(8)
N6^{i}—Zn1—O5^{ii}	88.32(8)		

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

Table S2. SHAPE analysis of Zn^{II} ion in **JXUST-3**.

ion	**label**	**shape**	**symmetry**	**distortion(τ)**
Zn1	HP-6	Hexagon	D_{6h}	29.441
	PPY-6	Pentagonal pyramid	C_{5v}	21.296
	OC-6	Octahedron	O_h	**5.228**
	TPR-6	Trigonal prism	D_{3h}	12.850
	JPPY-6	Johnson pentagonal pyramid J2	C_{5v}	25.308

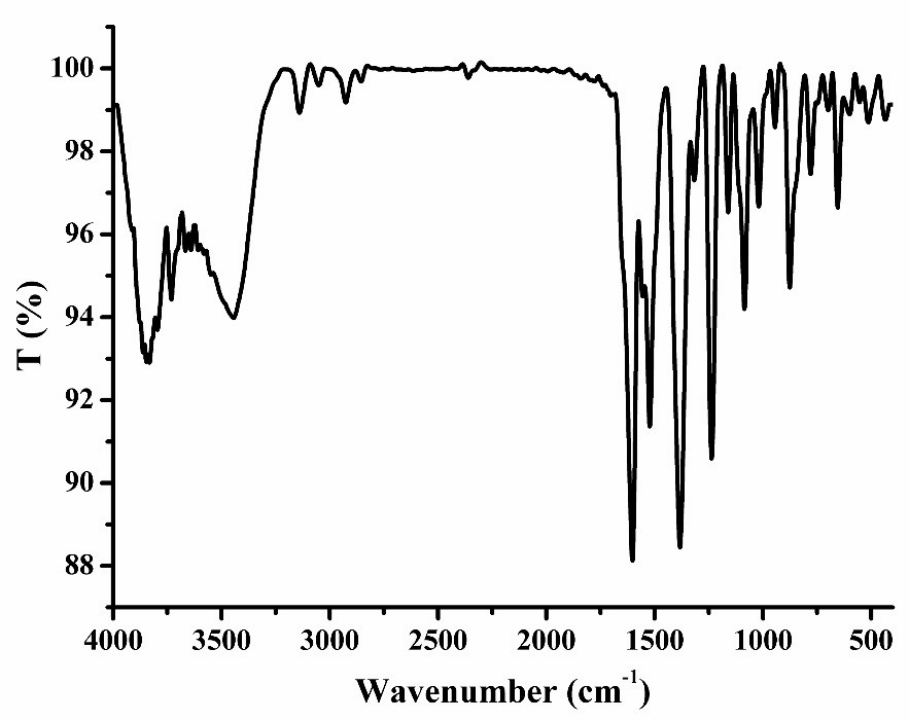


Fig. S1. IR spectrum of **JXUST-3** at room temperature.

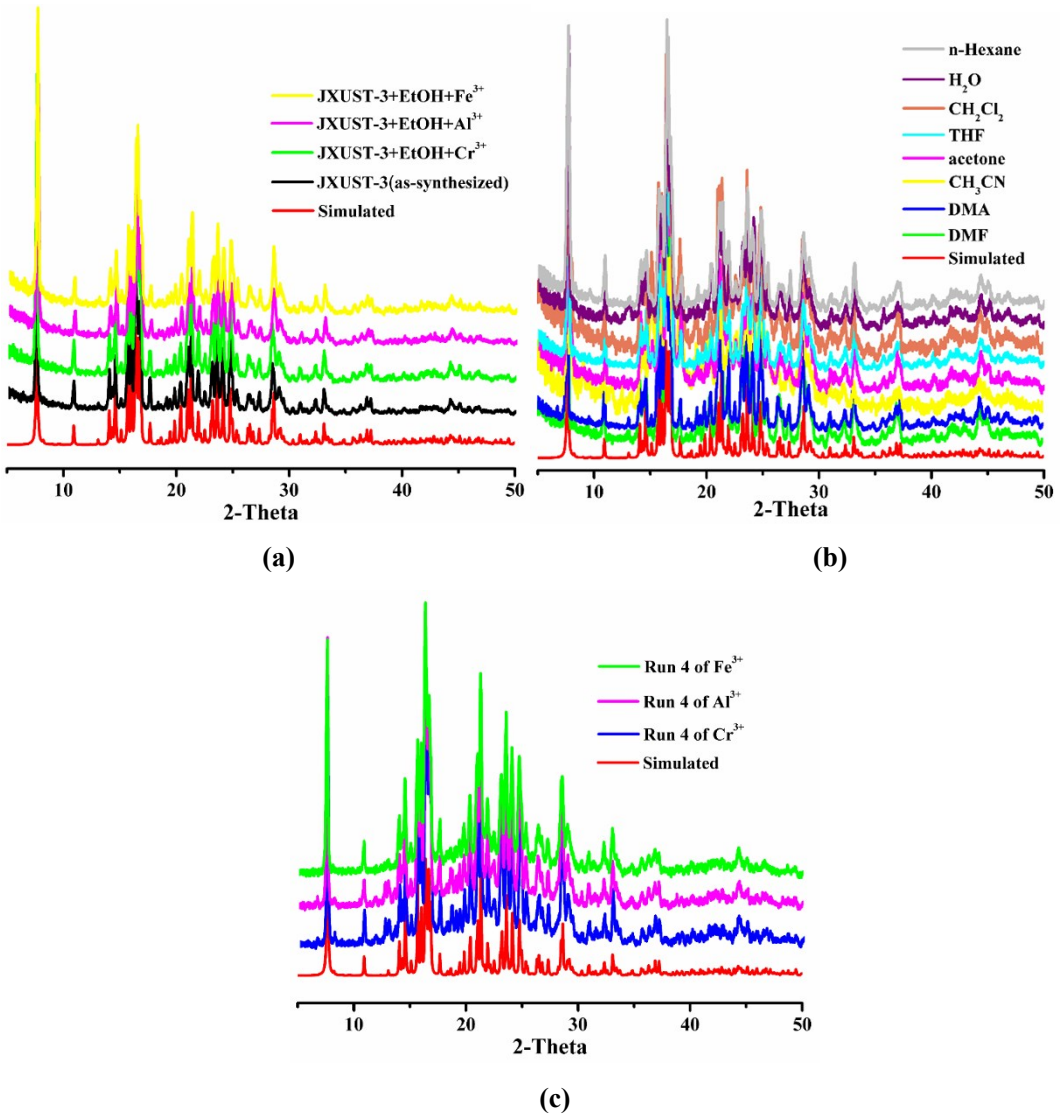


Fig. S2. (a) PXRD patterns of the simulated, as-synthesized sample, and samples after immersing in Cr^{3+}, Al^{3+} and Fe^{3+} EtOH solution for 16 h of **JXUST-3**; (b) PXRD patterns of **JXUST-3** after immersing in some common organic solvents for 24 h; (c) The PXRD patterns of **JXUST-3** after fluorescence recycling four times of Cr^{3+}, Al^{3+} and Fe^{3+}.

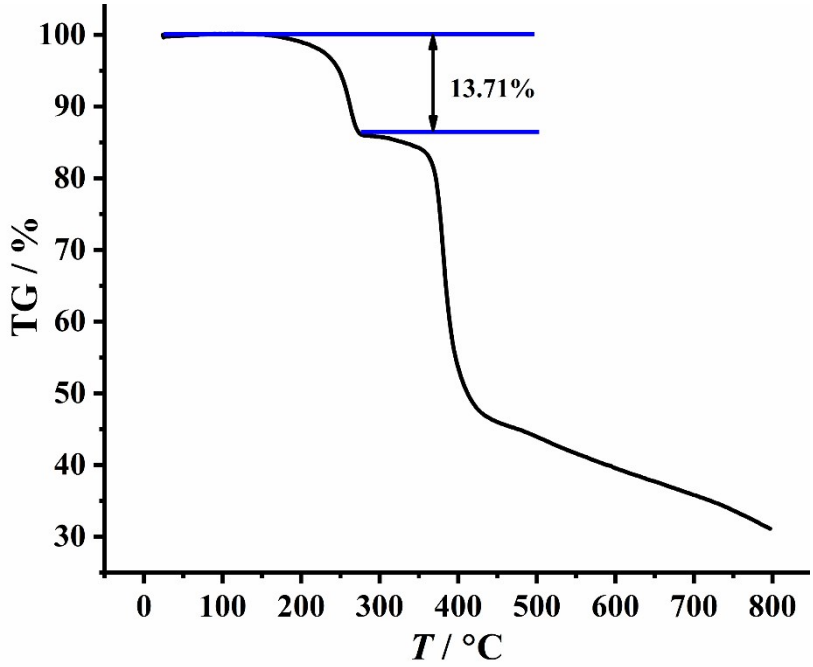


Fig. S3. The TGA curve of **JXUST-3** under N_2 atmosphere from room temperature to 800 °C.

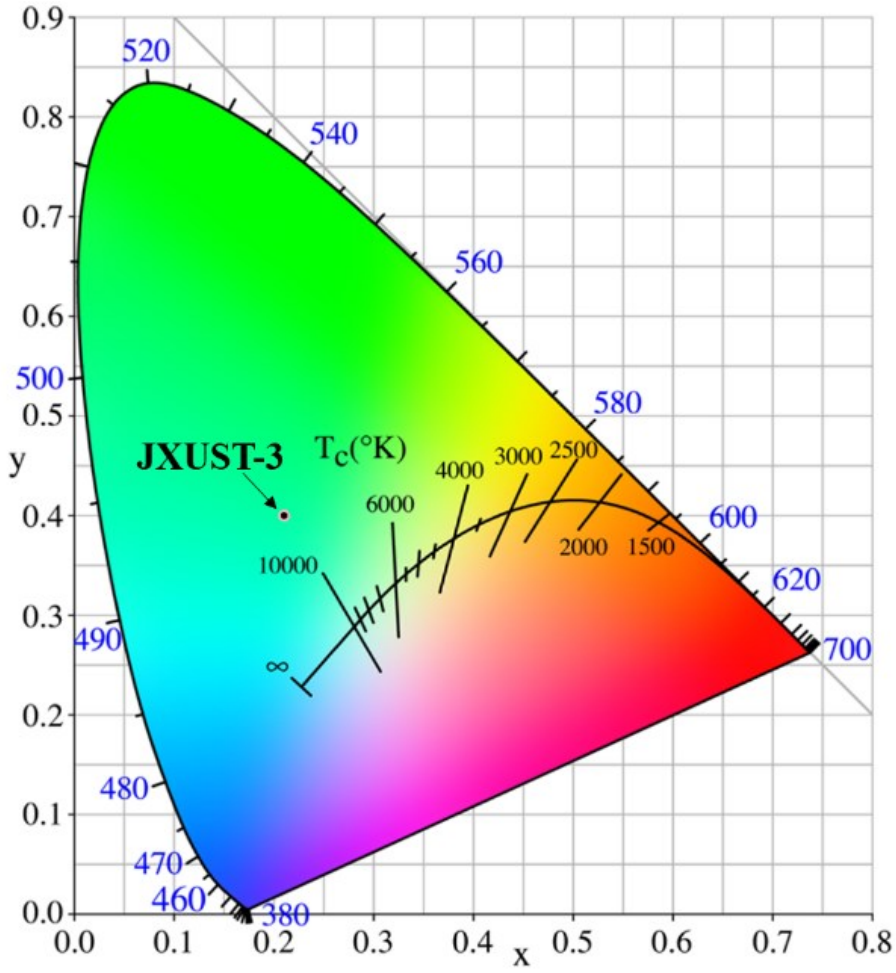


Fig. S4. CIE chromaticity diagram displaying the color coordinate of **JXUST-3**.

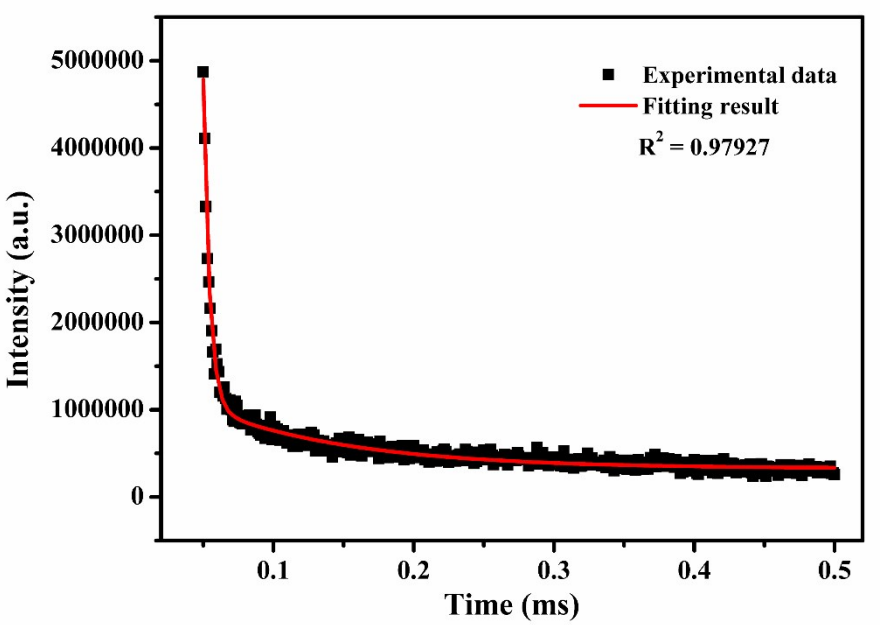


Fig. S5. The luminescence decay curve of **JXUST-3** at room temperature (λ_{ex} = 286 nm, λ_{em} = 492 nm).

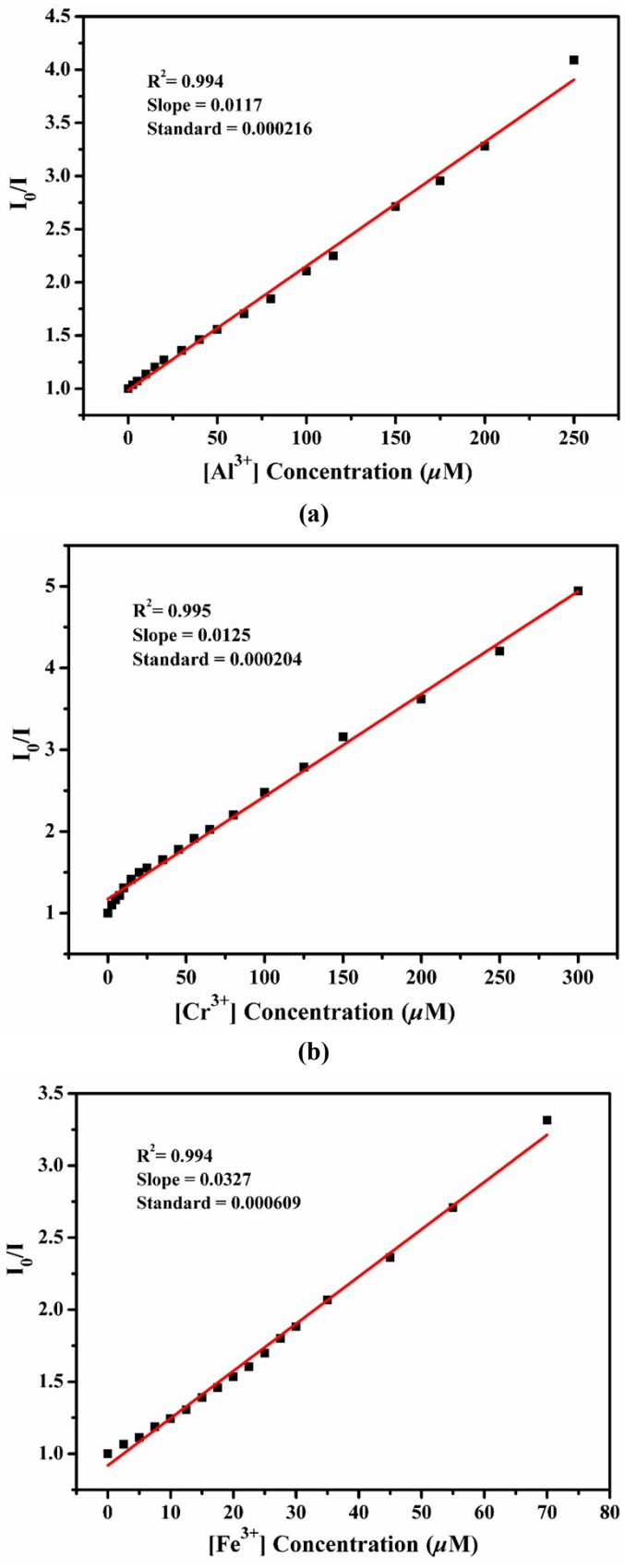
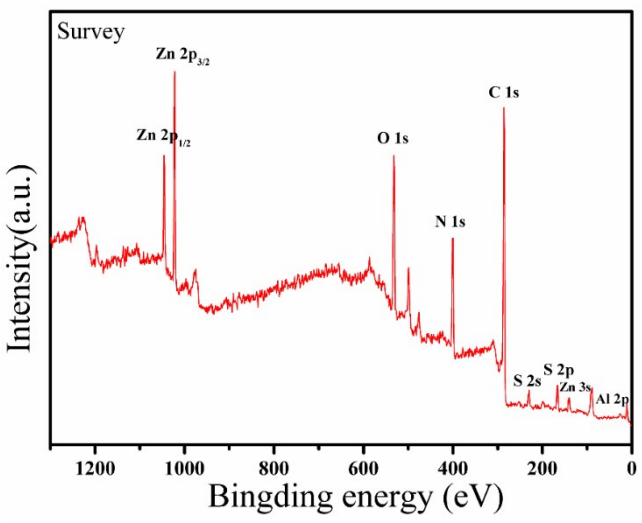
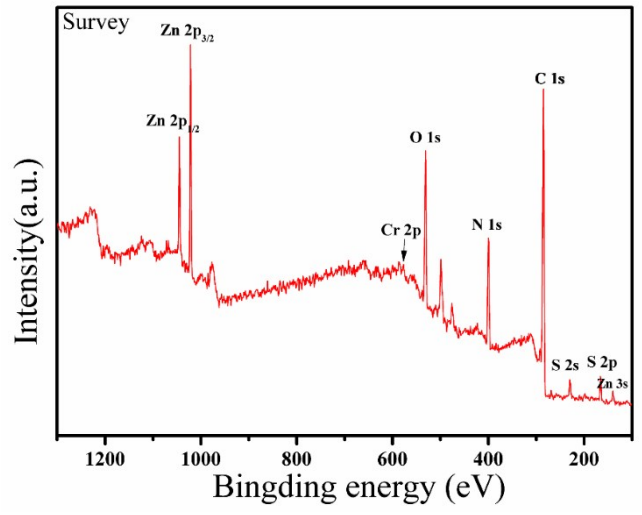


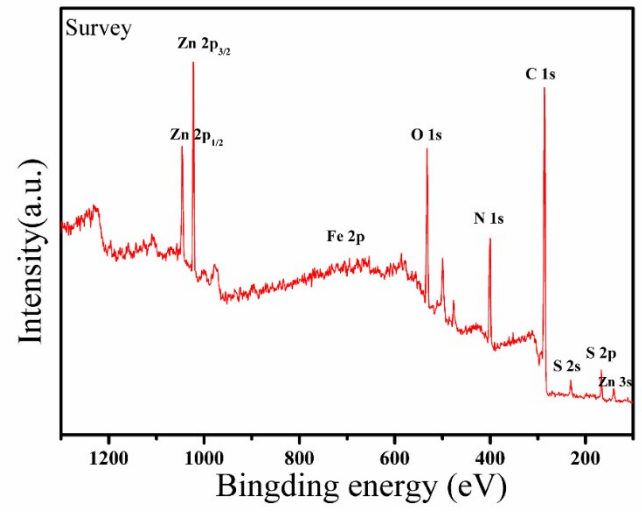
Fig. S6. Stern−Volmer plots of **JXUST-3** for Al^{3+} (a), Cr^{3+} (b) and Fe^{3+} (c).



(a)



(b)



(c)

Fig. S7. The XPS patterns of **JXUST-3** samples immersed in 0.3 mM Al^{3+} (a), Cr^{3+} (b), and Fe^{3+} (c) washed by ethanol five times.

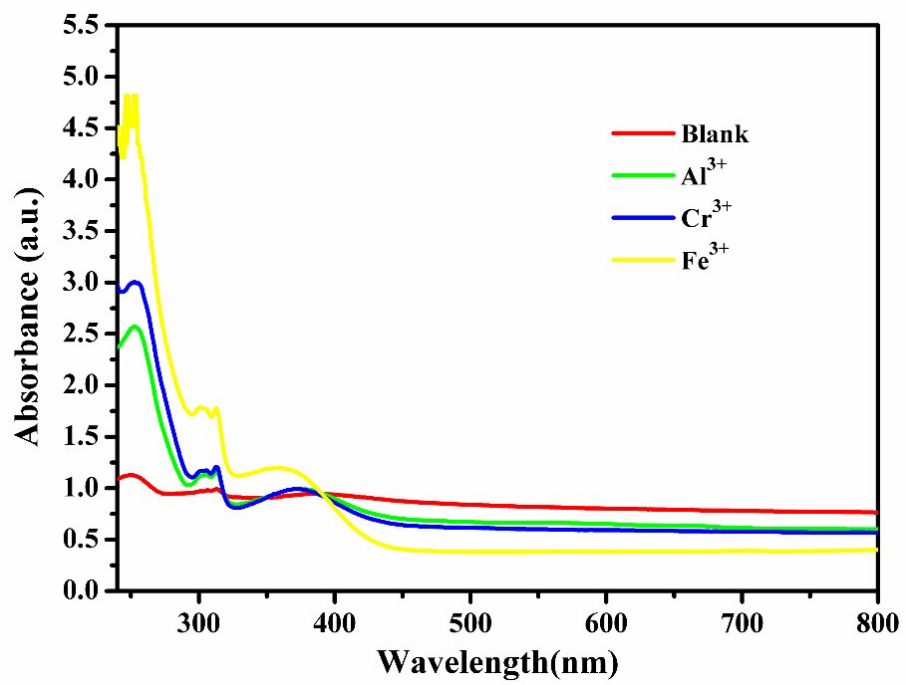


Fig. S8. UV-Vis absorption spectra of **JXUST-3** and **JXUST-3** upon the addition of Al^{3+}, Cr^{3+} and Fe^{3+} ions.