A simple fluorescent probe for selectively detecting Al^{3+} and F^- in cells and tea plant roots

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Fig. s1: ^1H NMR, ^{13}C NMR spectra of intermediate **BHMP**.

Fig. s2 (a) Changes of the fluorescence emission of **BHMP** + Al^{3+} on addition of different common anions (1. SO_4^{2-} 2. SO_3^{2-} 3. CO_3^{2-} 4. NO_3^- 5. F^- 6. Cl^- 7. Br^- 8. I^- 9. S^{2-} 10. $S_2O_3^{2-}$ 11. CH_3COO^- 12. PO_4^{3-} 13. HPO_4^{2-}). (b) Changes of the fluorescence intensity following the addition of $\mathbf{F^-}$ at different concentrations to the **BHMP+Al^{3+}**.

Fig. s3 (a) Job's plot between **BHMP** and Al^{3+} in CH_3CN. (b) Benesi-Hilderbrand plot of **BHMP** with Al^{3+} in CH_3CN.

Fig. s4 Fluorescence response time of **BHMP** to Al^{3+} in CH_3CN.

Fig. s5 HOMO, LUMO, and energy gap ($\Delta E = E_{HOMO} - E_{LUMO}$) of **BHMP** in Enol and Keto form calculated using the B3LYP function with 6-311G(d) basis set.

Fig. s6 the pH stability(a) of **BHMP** in PBS with different pH values and kinetic stability(b) in different solvents.

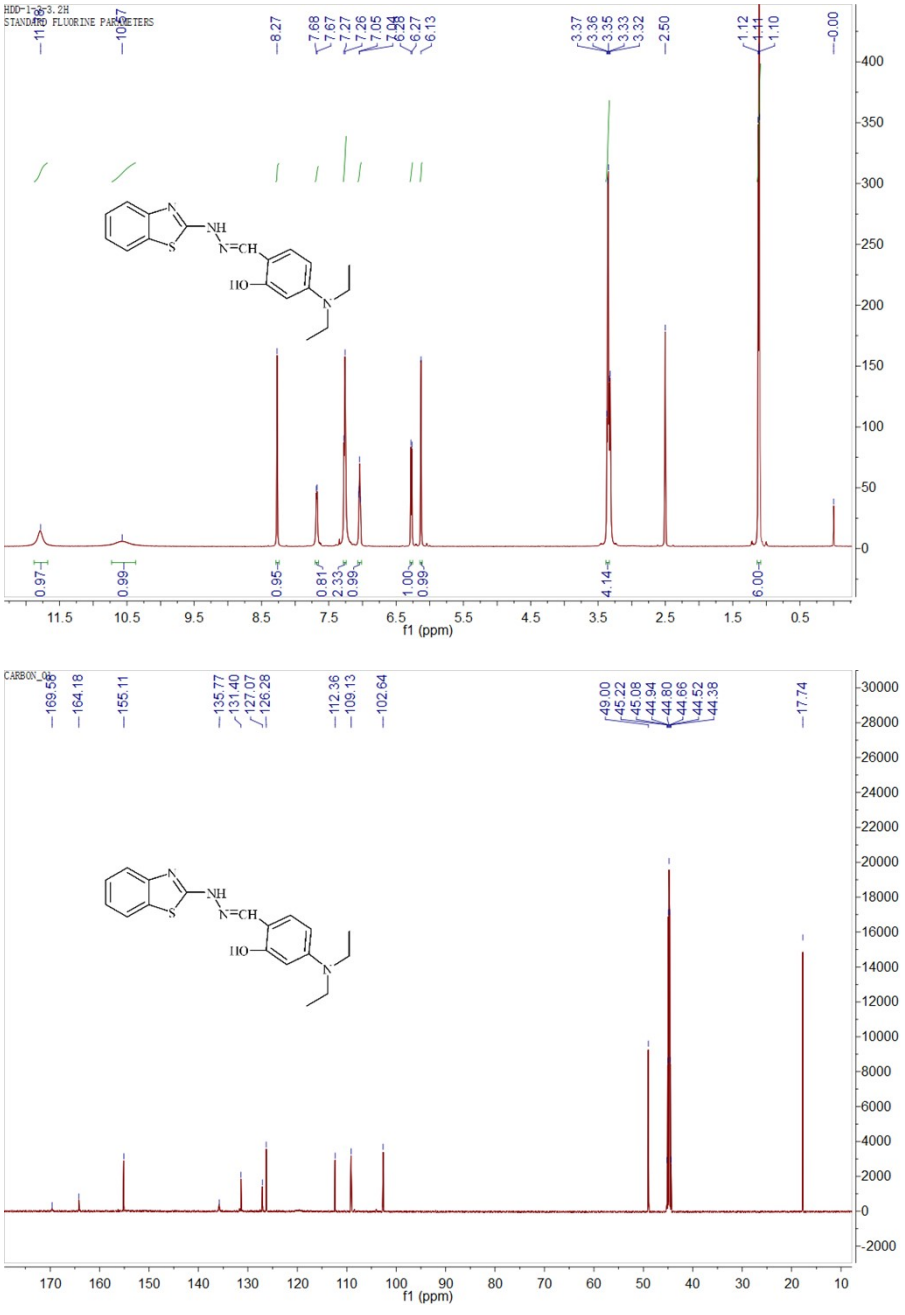
Fig. s7 MTT assays of Hela cells treated with **BHMP** at different concentrations for 24 h.

Table s1 the crystallographic data of **BHMP**

Table s2 Comparison of parameters between **BHMP** and other reported probes for Al^{3+} detection

Scheme s1 the synthetic routes of target compound **BHMP**.

Fig. s1 ^{1}H NMR and ^{13}C NMR spectra of intermediate **BHMP**.



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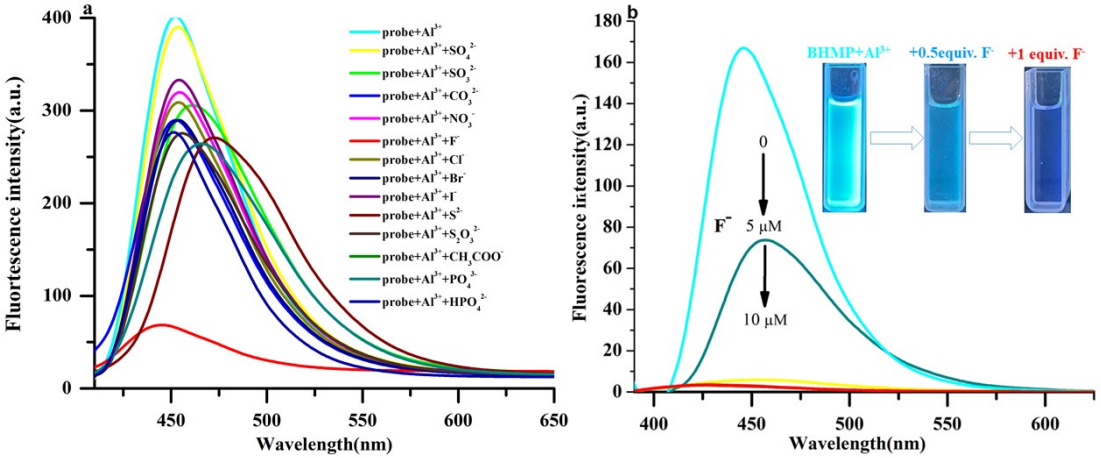

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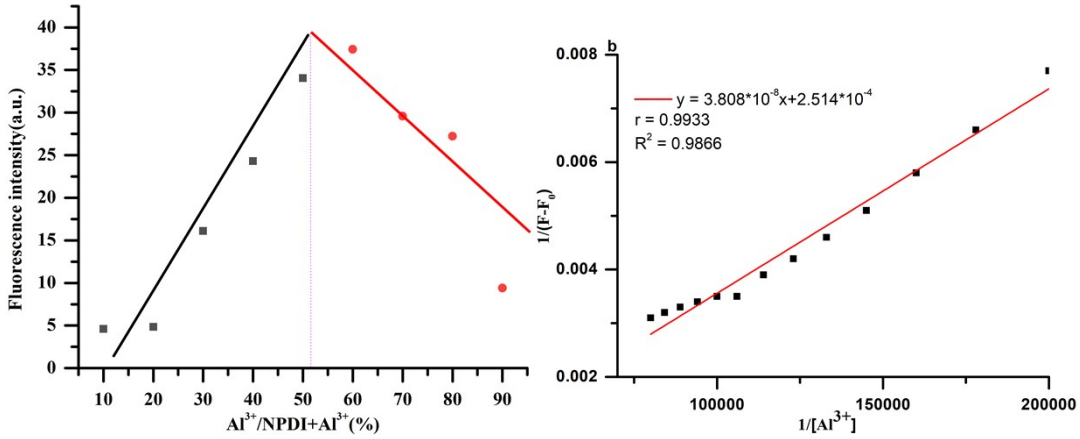

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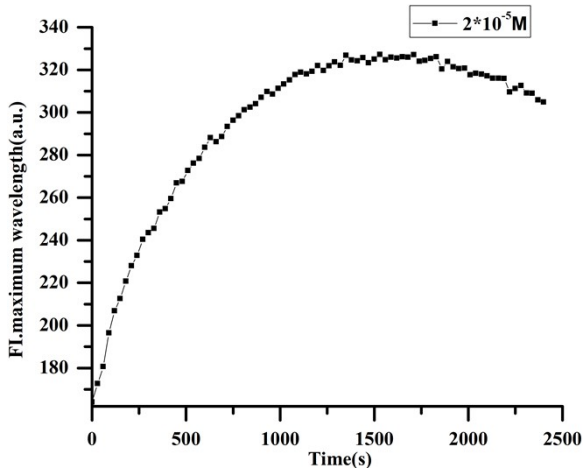

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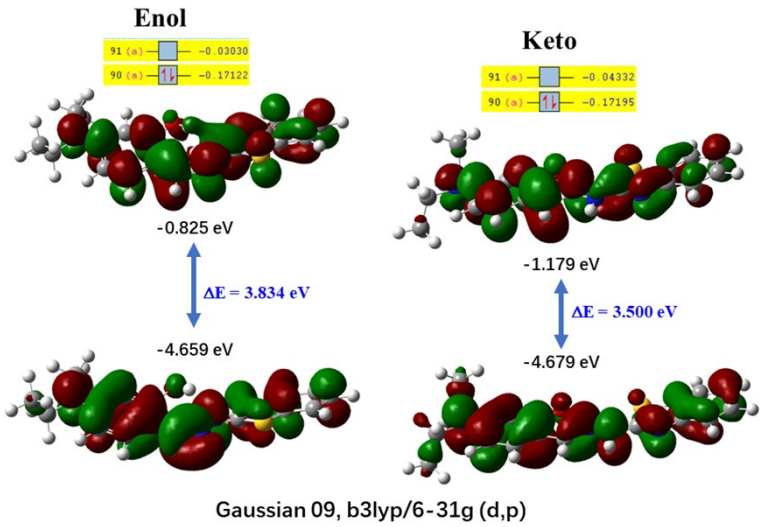

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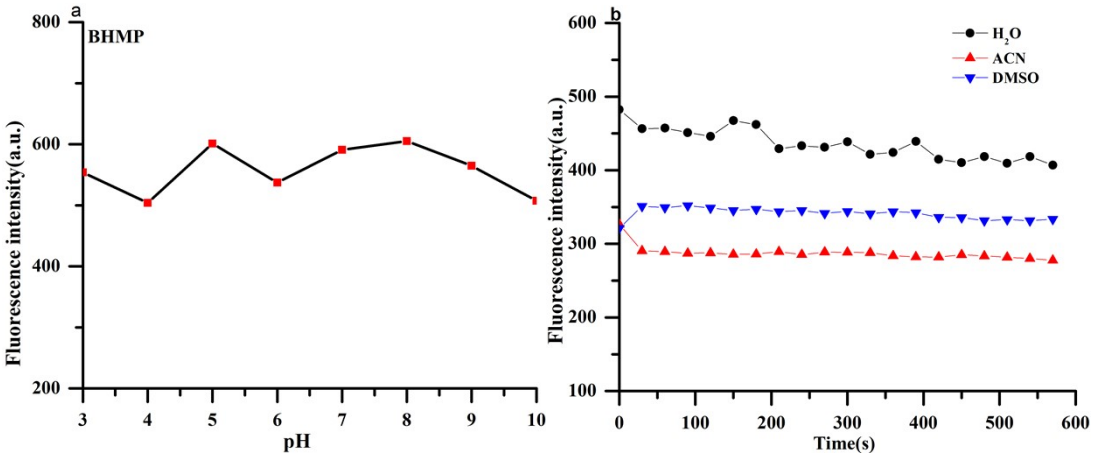

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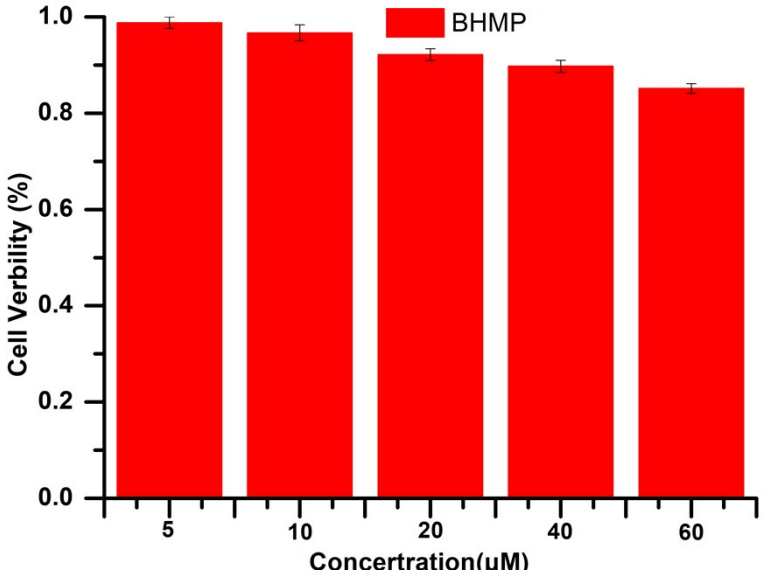

Table s1: The crystallographic data of **BHMP**

Compounds	**BHMP**
Empirical formula	$C_{18}H_{20}N_4OS$
Formula weight	340.44
Crystal system	Orthorhombic
Space group	Pccn
a[Å]	18.512(3)
b[Å]	27.014(4)
c[Å]	7.4371(12)
α[°]	90
β[°]	90
γ[°]	90
V[Å^3]	3719.2(10)
Z	8
T[K]	296
D_{calcd}[g·cm^{-1}]	1.216
F(000)	1440.0
μ[mm^{-1}]	0.185
θrange[°]	2.20-27.53
Total no. data	4014
No. unique data	1934
R_{int}	0.1512
R_1	0.0757
wR_2	0.2646
GOF	1.052

Table s2: Comparison of parameters between **BHMP** and other probes for Al^{3+} detection

Probe	λex (nm)	Medium (v:v)	Practical application	LOD (mol.L^{-1})	Ref.
Flu-py	523	Tris-HCl	Human cervical carcinoma cells	0.92×10^{-7} 1.12×10^{-7}	[8]
AHN	425	CH_3CN		1.148×10^{-6} 1.44×10^{-6}	[9]
SPBH	478	DMF:H_2O(1:1)	Human non-small cell lung cancer H460 cells	1.1×10^{-7} 1.47×10^{-6}	[10]
Probe1	540	CH_3CN:H_2O(9:1)	Water containing surfactant SDBS	3.2×10^{-8} 7.5×10^{-7}	[12]
H-2L	607	DMSO:H_2O(1:5)	A549 cells	1.05×10^{-8} 0.98×10^{-8}	[18]
BHMP	490	CH_3CN	Hela cells Tea plant roots	1.04×10^{-8}	This work

Scheme s1: The synthetic routes of target compound **BHMP**.