

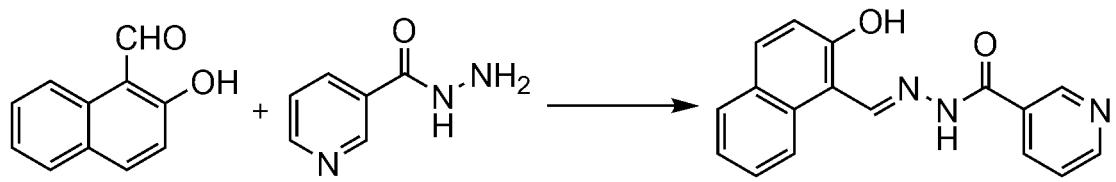
SUPPLEMENTARY MATERIAL

A Highly Selective and Sensitive Chemosensor for Colorimetric and Fluorescent Detection of Al³⁺ and Living Cell Imaging

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Scheme 1 Synthesis of HNN

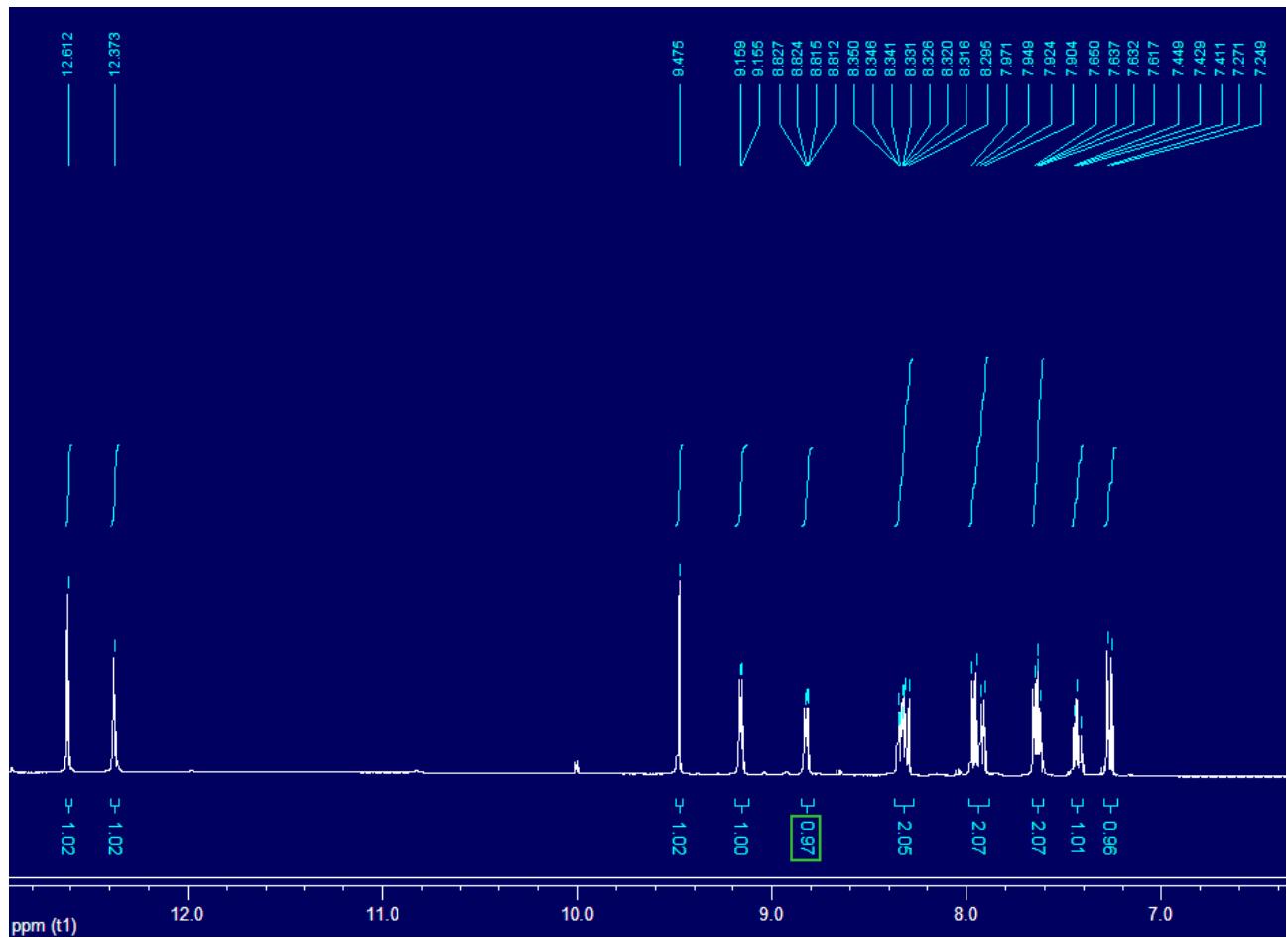


Fig. S1. ^1H NMR spectrum of HNN.

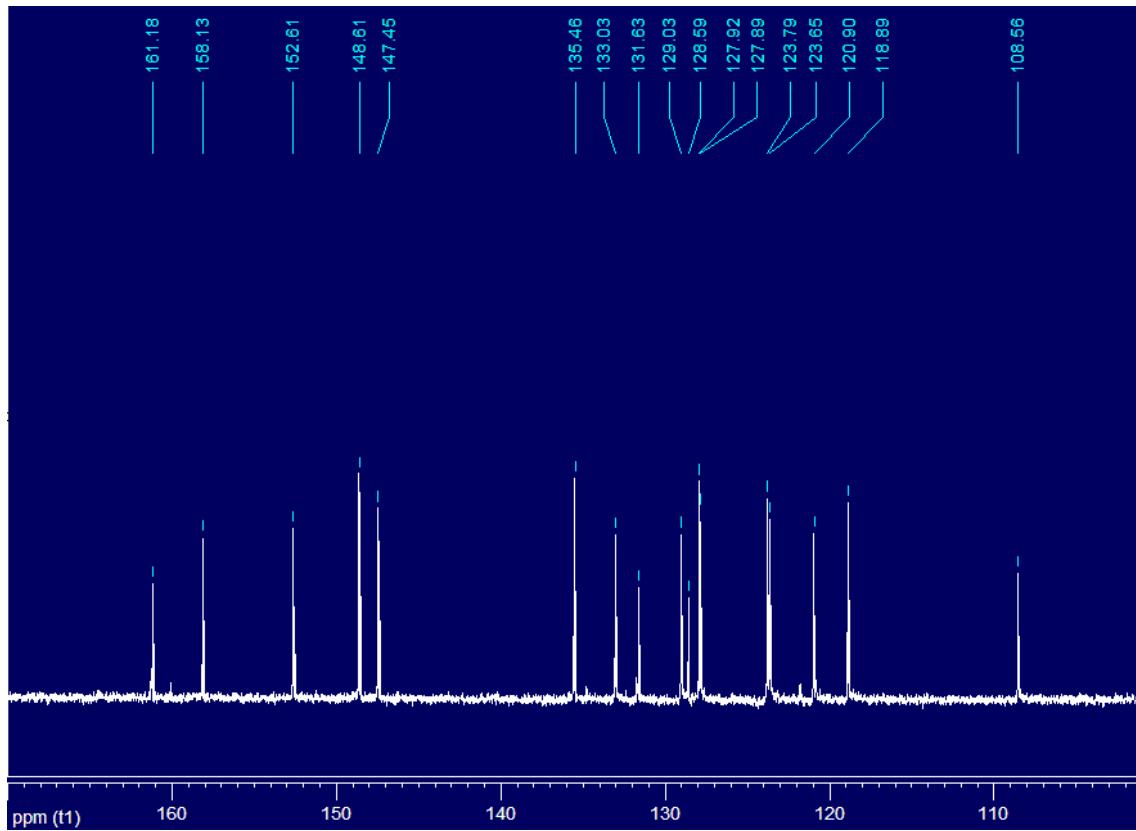


Fig. S2. ^{13}C NMR spectrum of compound **HNN**.

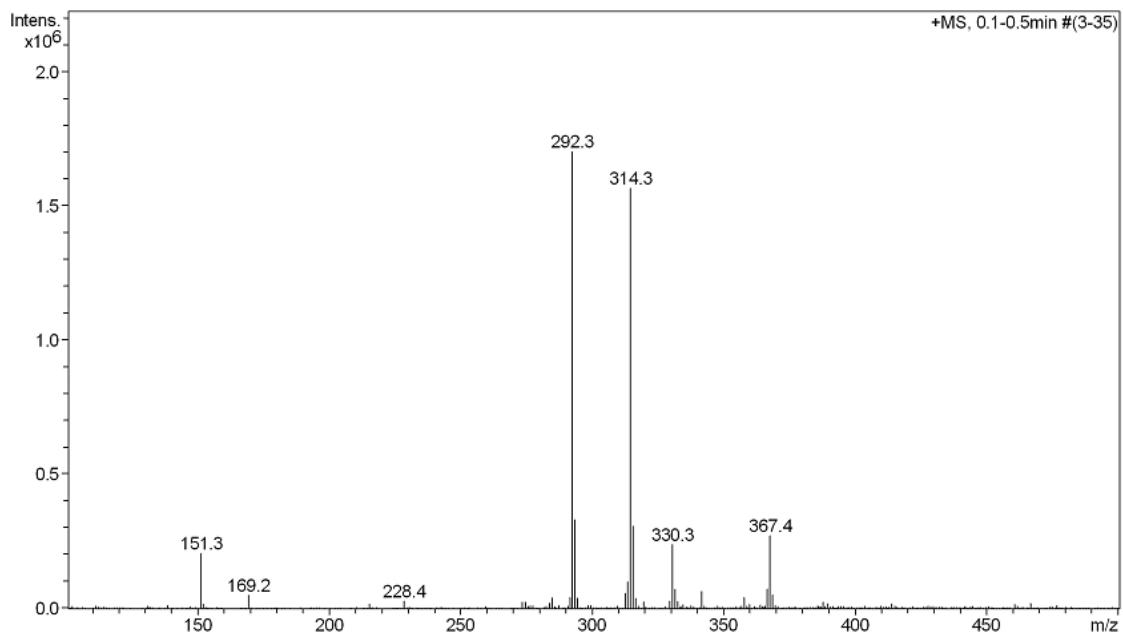


Fig. S3. ESI-MS spectrum of **HNN** in positive ion mode.
 $[\text{M}+\text{H}]^+$, $m/z = 292.3$; $[\text{M}+\text{Na}]^+$, $m/z = 314.3$; $[\text{M}+\text{K}]^+$, $m/z = 330.3$.

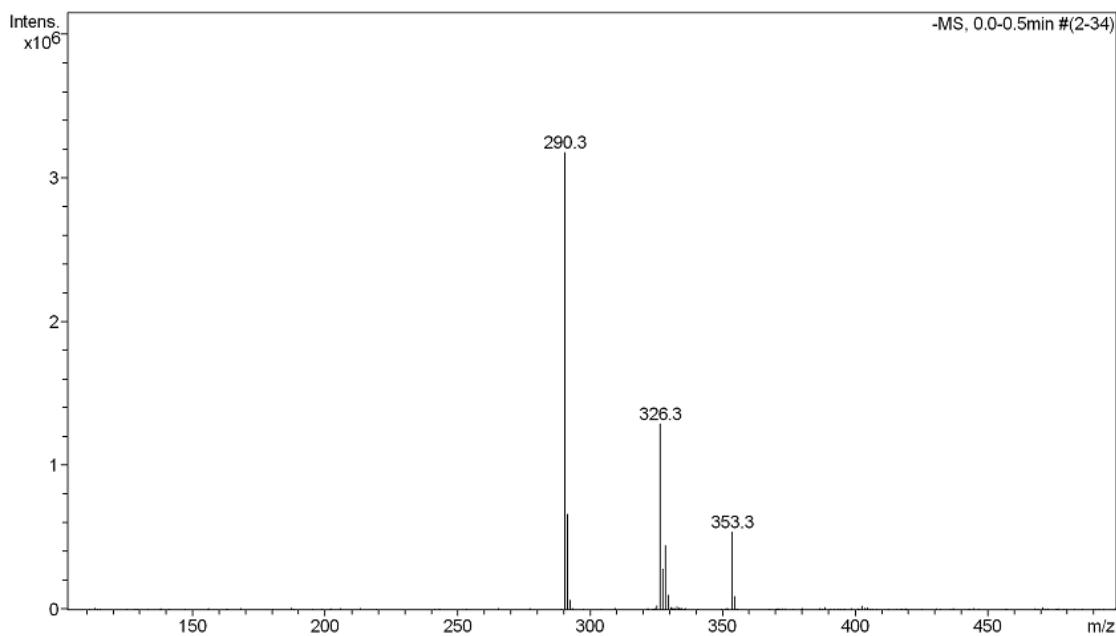


Fig. S4. ESI-MS spectrum of **HNN** in negative ion mode.
 $[\text{M}-\text{H}]$, m/z = 290.3; $[\text{M}+\text{H}_2\text{O}+\text{OH}]$, m/z = 326.3; $[\text{M}+\text{NO}_3]$, m/z = 353.3.

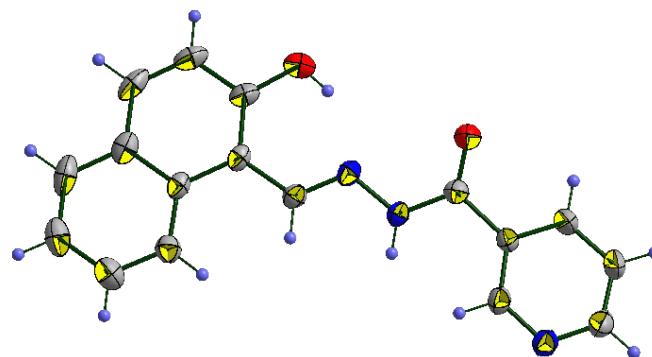


Fig. S5. The molecular structure of **HNN**. Thermal ellipsoids are shown at 30% probability levels.

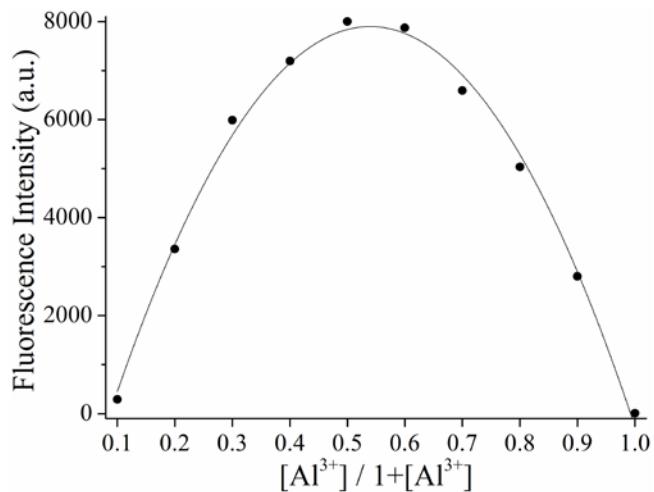


Fig. S6. Job's plot for **HNN/Al³⁺** in EtOH-H₂O (90/10, v/v) at 25 °C. The total $[\text{HNN}] + [\text{Al}^{3+}] = 40 \mu\text{M}$. $\lambda_{\text{ex}} = 410 \text{ nm}$, $\lambda_{\text{em}} = 480 \text{ nm}$.

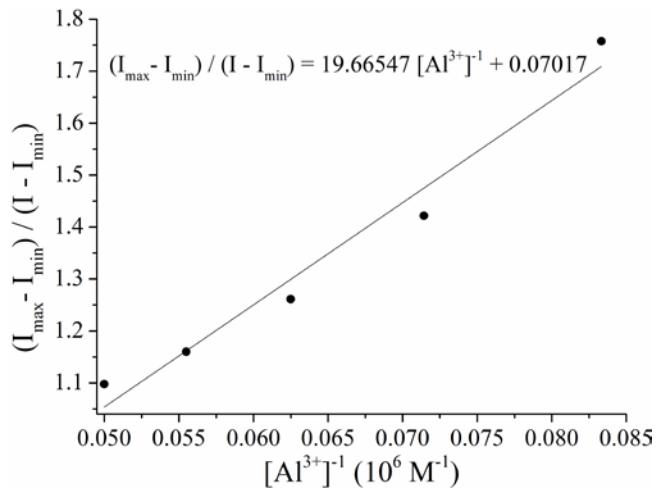


Fig. S7. Bensei-Hildebrand plot of $(I_{\max} - I_{\min}) / (I - I_{\min})$ as a function of $[Al^{3+}]^{-1}$ at $\lambda_{\text{ex}} = 410 \text{ nm}$, $\lambda_{\text{em}} = 480 \text{ nm}$.

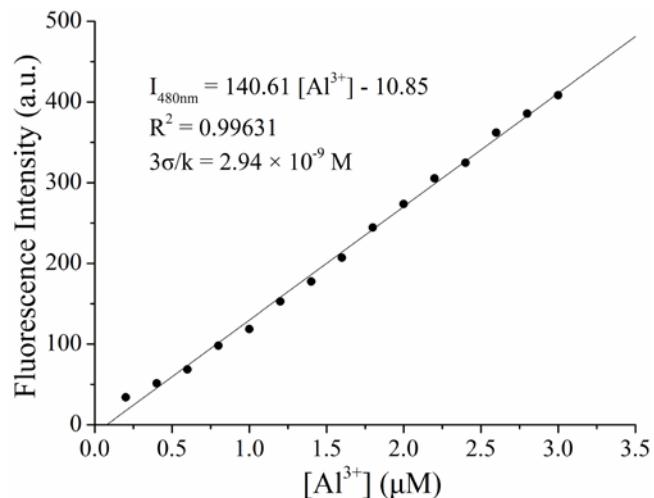


Fig. S8. Linear calibration curve of $I_{480\text{nm}}$ as a function of Al^{3+} concentration. $\lambda_{\text{ex}} = 410 \text{ nm}$, $\lambda_{\text{em}} = 480 \text{ nm}$.

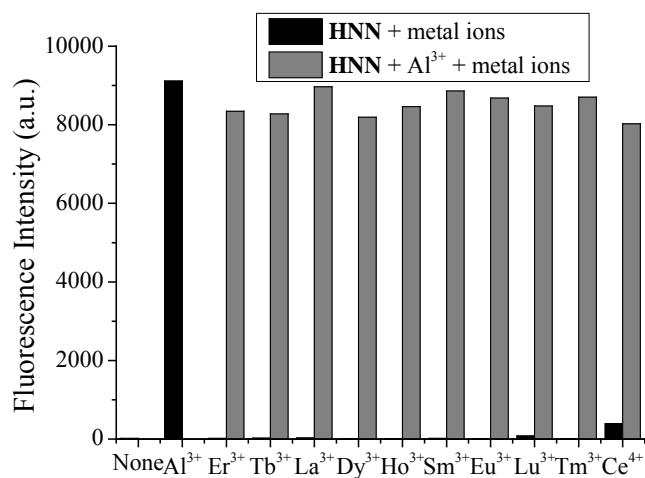


Fig. S9. The selective responses of HNN to Al^{3+} (2.0 equiv) in the presence of some rare-earth metal ions (2.0 equiv) at 480 nm.

Table 1. Crystal data and structure refinement

Empirical formula	C ₁₇ H ₁₃ N ₃ O ₂
Formula weight	291.30
Temperature/K	293(2)
Crystal system	orthorhombic
Space group	P2 ₁ 2 ₁ 2 ₁
<i>a</i> /Å	6.2664(5)
<i>b</i> /Å	12.3269(11)
<i>c</i> /Å	18.4866(12)
$\alpha/^\circ$	90.00
$\beta/^\circ$	90.00
$\gamma/^\circ$	90.00
Volume/Å ³	1428.0(2)
<i>Z</i>	4
$\rho_{\text{calc}}/\text{mg}\cdot\text{mm}^{-3}$	1.355
μ/mm^{-1}	0.092
<i>F</i> (000)	608.0
2 <i>θ</i> range/°	4.4 to 59.24
Index ranges	-8 ≤ <i>h</i> ≤ 6, -9 ≤ <i>k</i> ≤ 15, -17 ≤ <i>l</i> ≤ 25
Reflections collected	4675
Independent reflections	3083 [<i>R</i> (int)=0.0521]
Data/restraints/parameters	3083/0/200
Goodness-of-fit on <i>F</i> ²	1.017
<i>R</i> ₁ , <i>wR</i> ₂ [<i>I</i> >2σ(<i>I</i>)]	0.0726, 0.1237
<i>R</i> ₁ , <i>wR</i> ₂ [all data]	0.1670, 0.1641
Largest diff. peak / hole/ e·Å ⁻³	0.20/-0.22