## Supporting information

A fluorescence probe based on 6-phenylimidazo[2,1-b]thiazole and salicylaldehyde for relay discerning of $\mathrm{In}^{3+}$ and $\mathrm{Cr}^{3+}$ Bing Li, ${ }^{\text {a }}$ Xiaodong Shangb,*, Linlin Li, ${ }^{\text {a }}$ Yuankang $\mathrm{Xu},{ }^{\text {a }}$ Hanyu
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Fig.S1. ${ }^{1} \mathrm{H}$ NMR spectrum of compound 3.


Fig.S2. ${ }^{13} \mathrm{C}$ NMR spectrum of compound 3 .

| Sample Name | 190717-L-01 | Position | P1-F2 | Instrument Name | Instrument 1 | User Name |  |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| Inj Vol | -1 | InjPosition |  | SampleType | Sample | IRM Calibration Status | Success |
| Data Filename | 190717-L-01.d | ACQ Method | $0103 . \mathrm{m}$ | Comment |  | Acquired Time | 7/17/2019 12:13:23 AM |



Fig.S3.ESI mass spectrum of compound 3


Fig.S4.The FTIR spectra of compound $\mathbf{3}$


Fig.S5. ${ }^{1} \mathrm{H}$ NMR spectrum of $\mathbf{L B} 1$.


Fig.S6. ${ }^{13} \mathrm{C}$ NMR spectrum of LB1

| Sample Name | 190717-L-02 | Position | P1-E2 | Instrument Name | Instrument 1 | User Name |  |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| Inj Vol | -1 | InjPosition |  | SampleType | Sample | IRM Calibration Status | Success |
| Data Filename | 190717-L-02.d | ACQ Method | $0103 . \mathrm{m}$ | Comment |  | Acquired Time | 7/17/2019 12:46:35 AM |



Fig.S7.ESI mass spectrum of LB1


Fig.S8.The FTIR spectra of LB1


Fig.S9. Linear response of the emission intensity changes of LB1 with the concentration of $\operatorname{In}^{3+}$. Excitation is at 365 nm .


Fig.S10. Absorption spectra of $\mathbf{L B 1}\left(1 \times 10^{-5} \mathrm{M}\right)$ in $\mathrm{DMF} / \mathrm{H}_{2} \mathrm{O}(9: 1, \mathrm{v} / \mathrm{v})$ containing Tris ( 0.01 M , $\mathrm{pH}=7.4)$ buffer solution in the presence of various metal ions $\left(\mathrm{Mg}^{2+}, \mathrm{Cu}^{2+}, \mathrm{Co}^{2+}, \mathrm{Al}^{3+}, \mathrm{Hg}^{2+}, \mathrm{Ag}^{+}\right.$, $\mathrm{Mn}^{2+}, \mathrm{Ga}^{3+}, \mathrm{K}^{+}, \mathrm{Ca}^{2+}, \mathrm{Ni}^{2+}, \mathrm{Fe}^{3+}, \mathrm{Cd}^{2+}, \mathrm{Cr}^{3+}$ and $\mathrm{Zn}^{2+}$ )


Fig.S11. Job's plot of the LB1+In ${ }^{3+}$ complex in DMF/ $\mathrm{H}_{2} \mathrm{O}(9: 1, \mathrm{v} / \mathrm{v})$ containing Tris ( 0.01 M , $\mathrm{pH}=7.4$ ) at $25^{\circ} \mathrm{C}$. The total concentration of LB 1 and $\mathrm{In}^{3+}$ was 0.1 mM . Excitation is at 365 nm , and emission was monitored at 468 nm .


Fig.S12. Change ratio of $\left[\mathrm{LB} 1+\mathrm{In}^{3+}\right]\left(1 \times 10^{-5} \mathrm{M}\right)$ in DMF/ $\mathrm{H}_{2} \mathrm{O}(9: 1$, $\mathrm{v} / \mathrm{v}$, Tris $0.01 \mathrm{M}, \mathrm{pH}=7.4)$ upon titration with $\mathrm{Cr}^{3+}\left(1 \times 10^{-6} \mathrm{M}\right)$. Emission is monitored at 468 nm .

| Sample Name | 190720-LB-03 | Position | P1-E2 | Instrument Name | Instrument 1 | User Name |  |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| Inj Vol | -1 | InjPosition |  | SampleType | Sample | IRM Calibration Status | Success |
| Data Filename | $190720-$ LB-03.d | ACQ Method | $0103 . \mathrm{m}$ | Comment |  | Acquired Time | 7/20/2019 10:02:23 PM |



Fig.S13. ESI mass spectrum of complex $\left[\mathbf{L B} 1+\mathbf{I n}^{\mathbf{3 +}}\right]$.

(b)


Fig.S14. XYZ coordination of the optimized structure of $\mathbf{L B 1}$ (a) and $\mathbf{L B} 1+\mathbf{I n}^{\mathbf{3 +}}$ (b).

| Sample Name | 190720-L8-04 | Position | P1-D2 | Instrument Name | Instrument 1 | User Name |  |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| Inj Vol | -1 | InjPosition |  | SampleType | Sample | IRM Calibration Status | Success |
| Data Filename | $190720-$ L8-04.d | ACQ Method | $0103 . \mathrm{m}$ | Comment |  | Acquired Time | 7/20/2019 10:04:38 PM |



Fig.S15. ESI mass spectrum of complex $\left[\mathbf{L B} 1+\mathbf{C r}^{\mathbf{3 +}}\right]$.


Fig.S16. (a) XYZ coordination of the optimized structure of $\mathbf{L B} 1+\mathbf{C r}^{3+}$.(b) Energy graphic illustration of HOMO and LUMO orbital LB1+Cr ${ }^{3+}$

Table S1 Determination of the $\mathrm{In}^{3+}$ concentration in tap water samples

| sample | $\mathrm{In}^{3+}$ added | $\mathrm{In}^{3+}$ recovered | Recovery | RSD |
| :--- | :--- | :--- | :--- | :--- |
|  | $\left(\mathrm{mol} \mathrm{L}^{-1}\right)$ | $\left(\mathrm{mol} \mathrm{L}^{-1}\right)$ | $(\%)$ | $(\%)$ |


| 1 | $2 \times 10^{-5}$ | $2.1 \times 10^{-5}$ | 107.4 | 0.53 |
| :--- | :--- | :--- | :--- | :--- |
| 2 | $3 \times 10^{-5}$ | $3.1 \times 10^{-5}$ | 105.7 | 0.68 |
| 3 | $4 \times 10^{-5}$ | $3.9 \times 10^{-5}$ | 97.5 | 1.33 |

Table S2 Determination of the $\mathrm{Cr}^{3+}$ concentration in tap water samples

| sample | $\mathrm{Cr}^{3+}$ added <br> $\left(\mathrm{mol} \mathrm{L}^{-1}\right)$ | $\mathrm{Cr}^{3+}$ recovered <br> $\left(\mathrm{mol} \mathrm{L}^{-1}\right)$ | Recovery <br> $(\%)$ | RSD <br> $(\%)$ |
| :--- | :--- | :--- | :--- | :--- |
| 1 | $3 \times 10^{-5}$ | $3 \times 10^{-5}$ | 101.6 | 0.92 |
| 2 | $6 \times 10^{-5}$ | $6.3 \times 10^{-5}$ | 106.3 | 1.31 |
| 3 | $7 \times 10^{-5}$ | $6.9 \times 10^{-5}$ | 98.6 | 1.49 |

Table S3 Determination of the $\operatorname{In}^{3+}$ concentration in drink water samples

| sample | $\mathrm{In}^{3+}$ added <br> $\left(\mathrm{mol} \mathrm{L}^{-1}\right)$ | $\mathrm{In}^{3+}$ recovered <br> $\left(\mathrm{mol} \mathrm{L}^{-1}\right)$ | Recovery <br> $(\%)$ | RSD <br> $(\%)$ |
| :--- | :--- | :--- | :--- | :--- |
| 1 | $1 \times 10^{-5}$ | $1.0 \times 10^{-5}$ | 96.3 | 1.46 |
| 2 | $2 \times 10^{-5}$ | $2.1 \times 10^{-5}$ | 106.8 | 0.35 |
| 3 | $3 \times 10^{-5}$ | $3.2 \times 10^{-5}$ | 107.1 | 1.78 |

Table S4 Determination of the $\mathrm{Cr}^{3+}$ concentration in drink water samples

| sample | $\mathrm{Cr}^{3+}$ added <br> $\left(\mathrm{mol} \mathrm{L}^{-1}\right)$ | $\mathrm{Cr}^{3+}$ recovered <br> $\left(\mathrm{mol} \mathrm{L}^{-1}\right)$ | Recovery <br> $(\%)$ | RSD <br> $(\%)$ |
| :--- | :--- | :--- | :--- | :--- |
| 1 | $1 \times 10^{-5}$ | $1.0 \times 10^{-5}$ | 103.3 | 0.54 |
| 2 | $3 \times 10^{-5}$ | $2.9 \times 10^{-5}$ | 98.9 | 0.11 |
| 3 | $4 \times 10^{-5}$ | $3.7 \times 10^{-5}$ | 91.3 | 0.76 |

Table S5 Comparison of type of indium sensors and their detection limits

| Solvent system | Detection limit | Response | Reference |
| :--- | :--- | :--- | :--- |
| $\mathrm{CH}_{3} \mathrm{CN}$ | $1.9 \times 10^{-7} \mathrm{M}$ | turn-off | 5 |
| $\mathrm{CH}_{3} \mathrm{CN} / \mathrm{H}_{2} \mathrm{O}(\mathrm{v} / \mathrm{v}, 1: 1)$ | $7 \times 10^{-8} \mathrm{M}$ | off-on | 6 |
| Methanol $/ \mathrm{H}_{2} \mathrm{O}(\mathrm{v} / \mathrm{v}, 6: 4)$ | $1.4 \times 10^{-8} \mathrm{M}$ | - | 15 |
| Ethanol | $6.1 \times 10^{-7} \mathrm{M}$ | turn-on | 56 |
| DMF/ $\mathrm{H}_{2} \mathrm{O}(\mathrm{v} / \mathrm{v}, 9: 1)$ | $2.59 \times 10^{-9} \mathrm{M}$ | off-on | this work |

Table S6 Comparison of type of chromium sensors and their detection limits

| Solvent system | Detection limit | Response | Reference |
| :--- | :--- | :--- | :--- |
| DMF | $4.8 \times 10^{-6} \mathrm{M}$ | turn-off | 57 |
| $\mathrm{CH}_{3} \mathrm{CN} / \mathrm{HEPES}$ | $6.09 \times 10^{-6} \mathrm{M}$ | off-on | 58 |
| $\mathrm{CH}_{3} \mathrm{CN} / \mathrm{HEPES}(\mathrm{v} / \mathrm{v}, 4: 6)$ | $1 \times 10^{-6} \mathrm{M}$ | turn-on | 59 |
| DMF/Water(v/v,9:1) | $9 \times 10^{-6} \mathrm{M}$ | turn-off | 60 |
| DMSO/Methanol $(\mathrm{v} / \mathrm{v}, 9: 1)$ | $4 \times 10^{-4} \mathrm{M}$ | turn-on | 61 |
| $\mathrm{DMF} / \mathrm{H}_{2} \mathrm{O}(\mathrm{v} / \mathrm{v}, 9: 1)$ | $8.05 \times 10^{-7} \mathrm{M}$ | on-off | this work |

