Supporting Information For

A new quinoline based luminescent Zr(IV) metal-organic framework for the ultrasensitive recognition of 4-nitrophenol and Fe(III) ion

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Figure S1. EDX spectrum of 1'.

Table S1. Structural refinement parameters for 1 obtained from Rietveld refinement.

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Formula of activated sample</td>
<td>[\text{Zr}_6\text{O}_6\text{(OH)}_2(\text{CF}_3\text{COO})<em>2(\text{C}</em>{11}\text{H}_5\text{NO}_4)_4(\text{H}_2\text{O})_4]]</td>
</tr>
<tr>
<td>Crystal system</td>
<td>Orthorhombic</td>
</tr>
<tr>
<td>Space group</td>
<td>Immm</td>
</tr>
<tr>
<td>(a) / Å</td>
<td>11.673(2)</td>
</tr>
<tr>
<td>(b) / Å</td>
<td>17.688(3)</td>
</tr>
<tr>
<td>(c) / Å</td>
<td>25.498(3)</td>
</tr>
<tr>
<td>(V) / Å(^3)</td>
<td>5264(1)</td>
</tr>
<tr>
<td>(R_{wp}) / %</td>
<td>6.1</td>
</tr>
<tr>
<td>(R_p) / %</td>
<td>4.7</td>
</tr>
<tr>
<td>(R_{Bragg}) / %</td>
<td>1.7</td>
</tr>
<tr>
<td>GoF</td>
<td>3.3</td>
</tr>
</tbody>
</table>
**Figure S2.** FE-SEM image of 1.

**Figure S3.** XRPD patterns of calculated 1, as-synthesized 1 and thermally activated 1'.
Figure S4. FT-IR spectra of 1 (red) and 1' (black).

Figure S5. TG curve of as-synthesized 1 recorded in an argon atmosphere in the temperature range of 25-650 °C with a heating rate of 10 °C/min.
**Figure S6.** TG curve of activated 1\' recorded in an argon atmosphere in the temperature range of 25-650 °C with a heating rate of 10 °C/min.

**Figure S7.** XRPD patterns of 1 in different forms: (a) activated; (b) after 5 cycles of fluorescence titration experiments with 4-NP; (c) after 5 cycles of fluorescence titration experiments with Fe^{3+} ions; (d) after treatment with water; (e) after treatment with acetic acid; (f) after treatment with methanol; (g) after treatment with 1(M) HCl; (h) after BET analysis; (i) after treatment with 1(M) NaOH.
Figure S8. N$_2$ adsorption (filled circles) and desorption (empty circles) isotherms of thermally activated 1' measured at –196 °C.

Figure S9. Emission spectra of H$_2$QDA ligand (red, $\lambda_{ex} = 320$ nm) and compound 1' (black, $\lambda_{ex} = 320$ nm) measured in the solid state.
Figure S10. Fluorescence emission spectra of 1' in common organic solvents ($\lambda_{ex} = 320$ nm).

Figure S11. Quenching of the fluorescence intensity of 1' by incremental addition of 3 mM 2,4-DNP solution to a 3 mL suspension of 1' in acetonitrile.
Figure S12. Quenching of fluorescence intensity of 1' by incremental addition of 3 mM 2,4-DNT solution to a 3 mL suspension of 1' in acetonitrile.

Figure S13. Quenching of fluorescence intensity of 1' by incremental addition of 3 mM 2,6-DNT solution to a 3 mL suspension of 1' in acetonitrile.
Figure S14. Quenching of fluorescence intensity of 1' by incremental addition of 3 mM 2-NP solution to a 3 mL suspension of 1' in acetonitrile.

Figure S15. Quenching of fluorescence intensity of 1' by incremental addition of 3 mM 3-NP solution to a 3 mL suspension of 1' in acetonitrile.
**Figure S16.** Quenching of fluorescence intensity of 1' by incremental addition of 3 mM 4-NT solution to a 3 mL suspension of 1' in acetonitrile.

**Figure S17.** Quenching of fluorescence intensity of 1' by incremental addition of 3 mM 1,3-DNB solution to a 3 mL suspension of 1' in acetonitrile.
Figure S18. Quenching of fluorescence intensity of 1' by incremental addition of 3 mM NB solution to a 3 mL suspension of 1' in acetonitrile.

Figure S19. Quenching of fluorescence intensity of 1' by incremental addition of 3 mM TNP solution to a 3 mL suspension of 1' in acetonitrile.
Figure S20. Change in the fluorescence intensity of $1'$ upon addition of 3 mM 2,4-DNP solution (250 μL) in presence of 3 mM 4-NP (250 μL) solution.

Figure S21. Change in the fluorescence intensity of $1'$ upon addition of 3 mM 2,4-DNT solution (250 μL) in presence of 3 mM 4-NP (250 μL) solution.
Figure S22. Change in the fluorescence intensity of 1′ upon addition of 3 mM 2,6-DNT solution (250 µL) in presence of 3 mM 4-NP (250 µL) solution.

Figure S23. Change in the fluorescence intensity of 1′ upon addition of 3 mM 2-NP solution (250 µL) in presence of 3 mM 4-NP (250 µL) solution.
Figure S24. Change in the fluorescence intensity of 1' upon addition of 3 mM 3-NP solution (250 µL) in presence of 3 mM 4-NP (250 µL) solution.

Figure S25. Change in the fluorescence intensity of 1' upon addition of 3 mM 4-NT solution (250 µL) in presence of 3 mM 4-NP (250 µL) solution.
Figure S26. Change in the fluorescence intensity of 1’ upon addition of 3 mM 1,3-DNB solution (250 µL) in presence of 3 mM 4-NP (250 µL) solution.

Figure S27. Change in the fluorescence intensity of 1’ upon addition of 3 mM NB solution (250 µL) in presence of 3 mM 4-NP (250 µL) solution.
Figure S28. Change in the fluorescence intensity of 1' upon addition of 3 mM TNP solution (250 µL) in presence of 3 mM 4-NP (250 µL) solution.

Figure S29. Effect of other NAEs on the quenching efficiency of 4-NP.
**Figure S30.** Change of the fluorescence quenching efficiencies upon gradual addition of 3 mM solution of various nitroaromatic explosives to a 3 mL well-dispersed suspension of 1' in acetonitrile.

**Figure S31.** Recyclability test for the detection of 4-NP by 1'.
Figure S32. Quenching efficiencies of 1' as a function of exposure time.

Figure S33. Stern-Volmer plot for the quenching of 1' at lower concentrations of 4-NP. Inset: non-linearity of the Stern-Volmer plot at higher concentrations of 4-NP.
Table S2. A comparison of the Stern-Volmer constant ($K_{sv}$), detection limit and medium used for the detection of 4-NP by luminescent MOFs reported till date.

<table>
<thead>
<tr>
<th>Sl. No.</th>
<th>MOF</th>
<th>$K_{sv}$ (M$^{-1}$)</th>
<th>Detection Limit</th>
<th>Medium Used</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Zr$_6$O$_4$(OH)$_4$(CF$_3$COO)$<em>4$(C$</em>{11}$H$_5$NO$_4$)$_4$·10H$_2$O·3DMF</td>
<td>5.04×10$^9$</td>
<td>1.01×10$^{-11}$ M</td>
<td>acetonitrile</td>
<td>This work</td>
</tr>
<tr>
<td>2</td>
<td>[Zr$_6$O$_4$(OH)$_4$(2,7-CDC)$_6$]·19H$_2$O·2DMF</td>
<td>1.40×10$^4$</td>
<td>1.80×10$^{-8}$ M</td>
<td>THF</td>
<td>1</td>
</tr>
<tr>
<td>3</td>
<td>[Cu$<em>3$(L)$</em>{1.5}$(H$_2$O)$_3$]·3DEF·20H$_2$O (UPC-21)</td>
<td>3.10×10$^6$</td>
<td>89.6 ppb</td>
<td>DMSO</td>
<td>2</td>
</tr>
<tr>
<td>4</td>
<td>Ba$_5$(ADDA)$_3$(EtOH)$_2$(H$_2$O)$_3$·5DMF (UPC-17)</td>
<td>6.4×10$^6$ 2.27×10$^{-7}$ M</td>
<td>MeOH</td>
<td>3</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>8.9×10$^3$ 2.19×10$^{-7}$ M</td>
<td>acetone</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>1.26×10$^4$ 1.57×10$^{-7}$ M</td>
<td>THF</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>[Eu$_2$(L)$_3$(H$_2$O)$_3$]·2H$_2$O</td>
<td>2.20×10$^4$</td>
<td>-</td>
<td>DMSO</td>
<td>4</td>
</tr>
<tr>
<td>6</td>
<td>[Zr$_6$O$_4$(OH)$_8$(H$_2$O)$<em>4$(CTTA)$</em>{8/3}$] (BUT-12)</td>
<td>4.20×10$^4$</td>
<td>-</td>
<td>water</td>
<td>5</td>
</tr>
<tr>
<td>7</td>
<td>[Zr$_6$O$_4$(OH)$_8$(H$_2$O)$<em>4$(TTNA)$</em>{8/3}$] (BUT-13)</td>
<td>4.70×10$^4$</td>
<td>-</td>
<td>water</td>
<td>6</td>
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<tr>
<td>8</td>
<td>[Gd$_6$(L)$_3$(HL)$_2$(H$<em>2$O)$</em>{10}$]·18H$_2$O·x(solvent)</td>
<td>0.84 ×10$^4$</td>
<td>1.67 ppm</td>
<td>water</td>
<td>6</td>
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<tr>
<td>9</td>
<td>[Eu$_6$(L)$_3$(HL)$_2$(H$<em>2$O)$</em>{10}$]·10H$_2$O·x(solvent)</td>
<td>-</td>
<td>1.7×10$^{-6}$ M</td>
<td>water</td>
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<tr>
<td>10</td>
<td>[Cd$_4$(bptc)$_2$(DMA)$_4$(H$_2$O)$_2$·4DMA]</td>
<td>1.67×10$^5$</td>
<td>0.37 ppm</td>
<td>DMF</td>
<td>8</td>
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</table>
Figure S34. Lifetime decay profile of 1′ before and after addition of 300 µL of 3 mM 4-NP solution.

Table S3. Average excited-state lifetime (⟨τ⟩) values of 1′ before and after addition of 200 µL of 3 mM 4-NP solution (λ<sub>ex</sub> = 330 nm).

<table>
<thead>
<tr>
<th>Volume of PNP added (µL)</th>
<th>B&lt;sub&gt;1&lt;/sub&gt;</th>
<th>B&lt;sub&gt;2&lt;/sub&gt;</th>
<th>a&lt;sub&gt;1&lt;/sub&gt;</th>
<th>a&lt;sub&gt;2&lt;/sub&gt;</th>
<th>τ&lt;sub&gt;1&lt;/sub&gt; (ns)</th>
<th>τ&lt;sub&gt;2&lt;/sub&gt; (ns)</th>
<th>⟨τ⟩* (ns)</th>
<th>χ&lt;sup&gt;2&lt;/sup&gt;</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.023</td>
<td>0.006</td>
<td>0.36</td>
<td>0.64</td>
<td>0.87</td>
<td>6.30</td>
<td>4.36</td>
<td>1.00</td>
</tr>
<tr>
<td>200</td>
<td>0.030</td>
<td>0.004</td>
<td>0.41</td>
<td>0.59</td>
<td>0.46</td>
<td>5.28</td>
<td>3.29</td>
<td>1.00</td>
</tr>
</tbody>
</table>

* ⟨τ⟩ = a<sub>1</sub>τ<sub>1</sub> + a<sub>2</sub>τ<sub>2</sub>
**Figure S35.** Fluorescence intensity of 1' in acetonitrile as a function of 4-NP concentration.

**Figure S36.** HOMO and LUMO energies for the nitroaromatic explosives.
Table S4. HOMO and LUMO energy levels of selected analytes calculated by density functional theory (DFT) at B3LYP/6-31G* accuracy level using Gaussian 09 package of program.22

<table>
<thead>
<tr>
<th>Analytes</th>
<th>HOMO (eV)</th>
<th>LUMO (eV)</th>
<th>Band Gap (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>TNP</td>
<td>-8.2374</td>
<td>-3.898</td>
<td>4.3394</td>
</tr>
<tr>
<td>2,4-DNP</td>
<td>-7.6644</td>
<td>-2.8202</td>
<td>4.8442</td>
</tr>
<tr>
<td>4-NP</td>
<td>-6.9207</td>
<td>-2.2213</td>
<td>4.6994</td>
</tr>
<tr>
<td>4-NT</td>
<td>-7.3626</td>
<td>-2.3171</td>
<td>5.0455</td>
</tr>
<tr>
<td>2,4-DNT</td>
<td>-8.1131</td>
<td>-2.9769</td>
<td>5.1362</td>
</tr>
<tr>
<td>2,6-DNT</td>
<td>-7.8913</td>
<td>-2.8501</td>
<td>5.0412</td>
</tr>
<tr>
<td>1,3-DNB</td>
<td>-8.4129</td>
<td>-3.135</td>
<td>5.2779</td>
</tr>
<tr>
<td>NB</td>
<td>-7.5917</td>
<td>-2.4294</td>
<td>5.1623</td>
</tr>
</tbody>
</table>

Figure S37. Overlap between the absorption spectra of the nitroaromatic explosives and the emission spectrum of the acetonitrile suspension of 1′.
Figure S38. Change in the fluorescence intensity of 1’ upon incremental addition of 10 mM Al\textsuperscript{3+} solution in water.

Figure S39. Change in the fluorescence intensity of 1’ upon incremental addition of 10 mM Cd\textsuperscript{2+} solution in water.
Figure S40. Change in the fluorescence intensity of 1' upon incremental addition of 10 mM Co$^{2+}$ solution in water.

Figure S41. Change in the fluorescence intensity of 1' upon incremental addition of 10 mM Cr$^{3+}$ solution in water.
Figure S42. Change in the fluorescence intensity of 1' upon incremental addition of 10 mM Cu$^{2+}$ solution in water.

Figure S43. Change in the fluorescence intensity of 1' upon incremental addition of 10 mM Fe$^{2+}$ solution in water.
Figure S44. Change in the fluorescence intensity of I' upon incremental addition of 10 mM Hg$^{2+}$ solution in water.

Figure S45. Change in the fluorescence intensity of I' upon incremental addition of 10 mM K$^+$ solution in water.
Figure S46. Change in the fluorescence intensity of 1 upon incremental addition of 10 mM Mn$^{2+}$ solution in water.

Figure S47. Change in the fluorescence intensity of 1 upon incremental addition of 10 mM Na$^+$ solution in water.
Figure S48. Change in the fluorescence intensity of 1′ upon incremental addition of 10 mM Pb$^{2+}$ solution in water.

Figure S49. Change in the fluorescence intensity of 1′ upon incremental addition of 10 mM Ni$^{2+}$ solution in water.
Figure S50. Change in the fluorescence intensity of I’ upon incremental addition of 10 mM Zn$^{2+}$ solution in water.

Figure S51. Change in the fluorescence intensity of I’ upon addition of 10 mM Al$^{3+}$ solution (500 µL) in presence of 10 mM Fe$^{3+}$ (500 µL) solution in water.
Figure S52. Change in the fluorescence intensity of 1’ upon addition of 10 mM Cd$^{2+}$ solution (500 µL) in presence of 10 mM Fe$^{3+}$ (500 µL) solution in water.

Figure S53. Change in the fluorescence intensity of 1’ upon addition of 10 mM Co$^{2+}$ solution (500 µL) in presence of 10 mM Fe$^{3+}$ (500 µL) solution in water.
Figure S54. Change in the fluorescence intensity of 1’ upon addition of 10 mM Cr$^{3+}$ solution (500 µL) in presence of 10 mM Fe$^{3+}$ (500 µL) solution in water.

Figure S55. Change in the fluorescence intensity of 1’ upon addition of 10 mM Fe$^{2+}$ solution (500 µL) in presence of 10 mM Fe$^{3+}$ (500 µL) solution in water.
Figure S56. Change in the fluorescence intensity of $1'$ upon addition of 10 mM Hg$^{2+}$ solution (500 µL) in presence of 10 mM Fe$^{3+}$ (500 µL) solution in water.

Figure S57. Change in the fluorescence intensity of $1'$ upon addition of 10 mM K$^+$ solution (500 µL) in presence of 10 mM Fe$^{3+}$ (500 µL) solution in water.
Figure S58. Change in the fluorescence intensity of 1’ upon addition of 10 mM Mn$^{2+}$ solution (500 µL) in presence of 10 mM Fe$^{3+}$ (500 µL) solution in water.

Figure S59. Change in the fluorescence intensity of 1’ upon addition of 10 mM Na$^{+}$ solution (500 µL) in presence of 10 mM Fe$^{3+}$ (500 µL) solution in water.
Figure S60. Change in the fluorescence intensity of 1’ upon addition of 10 mM Ni$^{2+}$ solution (500 µL) in presence of 10 mM Fe$^{3+}$ (500 µL) solution in water.

Figure S61. Change in the fluorescence intensity of 1’ upon addition of 10 mM Pb$^{2+}$ solution (500 µL) in presence of 10 mM Fe$^{3+}$ (500 µL) solution in water.
**Figure S62.** Change in the fluorescence intensity of $1'$ upon addition of 10 mM Zn$^{2+}$ solution (500 µL) in presence of 10 mM Fe$^{3+}$ (500 µL) solution in water.

**Figure S63.** Effect of other metal cations on the quenching efficiency of Fe$^{3+}$ ion in water.
Figure S64. Change in the fluorescence intensity of 1’ in HEPES buffer (10 mM, pH = 7.4) upon incremental addition of 10 mM Fe$^{3+}$ solution.

Figure S65. The fluorescence quenching efficiencies of various metal cations (500 μL of 10 mM solution) towards 1’ suspended in HEPES buffer (10 mM, pH = 7.4).
Figure S66. Effect of other metal cations on the quenching efficiency of Fe$^{3+}$ ion in HEPES buffer (10 mM, pH = 7.4).

Figure S67. Reproducibility test for the aqueous suspension of 1 towards sensing of Fe$^{3+}$ ion.
**Figure S68.** Quenching efficiencies of 1' as a function of exposure time in water.

**Figure S69.** Change of fluorescence quenching efficiencies upon gradual addition of 10 mM solution of various metal cations to a 3 mL well-dispersed suspension of 1' in water.
**Figure S70.** Quenching efficiencies of 1' in HEPES buffer (10 mM, pH = 7.4) as a function of exposure time.

**Figure S71.** Stern-Volmer plot for the quenching of 1' at lower concentrations of Fe$^{3+}$ ion in water. Inset: non linearity of the Stern-Volmer plot at higher concentrations of Fe$^{3+}$ ion.
Figure S72. Stern-Volmer plot for the quenching of 1' at lower concentrations of Fe$^{3+}$ ion in HEPES buffer (10 mM, pH=7.4).

Table S5. A comparison of the Stern-Volmer constant ($K_{sv}$), detection limit and medium used for Fe$^{3+}$ detection for MOFs reported till date.

<table>
<thead>
<tr>
<th>Sl. No.</th>
<th>MOF</th>
<th>$K_{sv}$ (M$^{-1}$)</th>
<th>Detection Limit</th>
<th>Medium Used</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>[Zr$_6$O$_6$(OH)$_2$(CF$_3$COO)$<em>2$(C$</em>{11}$H$_5$NO$_4$)$_4$(H$_2$O)$_4$]</td>
<td>2.25×10$^7$</td>
<td>1.7×10$^{-9}$ M</td>
<td>Water</td>
<td>This work</td>
</tr>
<tr>
<td>2.</td>
<td>[Zr$_6$O$_6$(OH)$_2$(CF$_3$COO)$<em>2$(C$</em>{11}$H$_5$NO$_4$)$_4$(H$_2$O)$_4$]</td>
<td>1.91×10$^7$</td>
<td>2.7×10$^{-9}$ M</td>
<td>HEPES buffer</td>
<td>This work</td>
</tr>
<tr>
<td>3.</td>
<td>[La(TPT)(DMSO)$_2$]·H$_2$O</td>
<td>1.36×10$^4$</td>
<td>-</td>
<td>ethanol</td>
<td>9</td>
</tr>
<tr>
<td>4.</td>
<td>[H(H$_2$O)$_8$][DyZn$_4$(imdc)$_4$(im)$_4$]</td>
<td>2.88×10$^4$</td>
<td>-</td>
<td>DMSO</td>
<td>10</td>
</tr>
<tr>
<td>5.</td>
<td>EuL$_3$</td>
<td>4.1×10$^3$</td>
<td>10$^{-4}$ M</td>
<td>ethanol</td>
<td>11</td>
</tr>
<tr>
<td>6.</td>
<td>[Eu$_2$(MFDA)$_2$(HCOO)$_2$(H$_2$O)$_6$]·H$_2$O</td>
<td>-</td>
<td>3.3×10$^{-7}$ M</td>
<td>DMF</td>
<td>12</td>
</tr>
<tr>
<td>7.</td>
<td>[Cd(H$<em>2$L$</em>{a,5}$)(H$<em>2$L)$</em>{b,5}$(H$_2$O)]</td>
<td>-</td>
<td>10$^{-5}$ M</td>
<td>water</td>
<td>13</td>
</tr>
<tr>
<td>8.</td>
<td>[(CH$_3$)$_3$NH$_2$]·[Tb(bptc)]·xsolvents</td>
<td>-</td>
<td>72.76 ppm</td>
<td>ethanol</td>
<td>14</td>
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<tr>
<td>9.</td>
<td>[Ln$_2$(Cebp)$_3$·6H$_2$O]·3Cl·4H$_2$O</td>
<td>1.143×10$^5$</td>
<td>-</td>
<td>ethanol</td>
<td>15</td>
</tr>
<tr>
<td>10.</td>
<td>Eu$^{3+}$@MIL-124</td>
<td>3.87×10$^4$</td>
<td>0.28×10$^{-6}$ M</td>
<td>water</td>
<td>16</td>
</tr>
<tr>
<td>11.</td>
<td>MIL-53(Al)</td>
<td>-</td>
<td>0.9×10$^{-6}$ M</td>
<td>PBS buffer</td>
<td>17</td>
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<tr>
<td>12.</td>
<td>[Ln(Hpzbc)$_3$(NO$_3$)]·H$_2$O</td>
<td>-</td>
<td>2.6×10$^{-5}$ M</td>
<td>ethanol</td>
<td>18</td>
</tr>
<tr>
<td>13.</td>
<td>[Tb(BTB)(DMF)]·1.5DMF·2.5H$_2$O</td>
<td>-</td>
<td>10$^{-5}$ M</td>
<td>ethanol</td>
<td>19</td>
</tr>
</tbody>
</table>
14. [Tb$_4$(OH)$_4$(DSOA)$_2$(H$_2$O)$_8$](H$_2$O)$_8$ | 3.5×10$^4$ | - | water | 20
15. Tb$^{3+}$@Cd-MOF | 1.108×10$^5$ | 0.010 mM DMF | 21
16. [Zr$_6$O$_4$(OH)$_4$(2,7-CDC)$_6$] | 5.5×10$^3$ | 9.10×10$^{-7}$ M | water | 1

**Figure S73.** Lifetime decay profile of 1' before and after addition of 200 µL of 10 mM Fe$^{3+}$ solution in water.

**Table S6.** Average excited state lifetime ($<\tau>$) values of 1' before and after addition of 300 µL of 10 mM Fe$^{3+}$ solution ($\lambda_{ex} = 330$ nm).

<table>
<thead>
<tr>
<th>Volume of Fe$^{3+}$ solution added (µL)</th>
<th>B$_1$</th>
<th>B$_2$</th>
<th>a$_1$</th>
<th>a$_2$</th>
<th>$\tau_1$ (ns)</th>
<th>$\tau_2$ (ns)</th>
<th>$&lt;\tau&gt;^*$ (ns)</th>
<th>$\chi^2$</th>
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</thead>
<tbody>
<tr>
<td>0</td>
<td>0.068</td>
<td>0.014</td>
<td>0.10</td>
<td>0.90</td>
<td>0.35</td>
<td>14.68</td>
<td>13.20</td>
<td>1.09</td>
</tr>
<tr>
<td>300</td>
<td>0.144</td>
<td>0.002</td>
<td>0.69</td>
<td>0.31</td>
<td>0.22</td>
<td>7.99</td>
<td>2.60</td>
<td>0.92</td>
</tr>
</tbody>
</table>

* $<\tau> = a_1\tau_1 + a_2\tau_2$
Figure S74. Fluorescence intensity of 1' in water as a function of Fe$^{3+}$ concentration.

Figure 75. Fluorescence intensity of 1' in HEPES buffer (10 mM, pH = 7.4) as a function of Fe$^{3+}$ concentration.
**Figure S76.** EDX spectrum of 1' after treatment with 10 mM Fe$^{3+}$ aqueous solution.

**Figure S77.** UV-Vis absorption spectra of the aqueous solutions containing different metal ions (10×10^{-3} M). The emission spectra of 1' (pink color) (3 mg) dispersed in water (3 mL).
Calculated Crystallographic Information File (CIF) for compound 1:

data_compound 1
_chemical_name_mineral ??
_cell_length_a  11.6730(20)
_cell_length_b  17.6881(29)
_cell_length_c  25.4979(34)
_cell_angle_alpha 90
_cell_angle_beta  90
_cell_angle_gamma 90
_cell_volume 5264.6(14)
_symmetry_space_group_name_H-M IMMM
loop_
_symmetry_equiv_pos_as_xyz
' -x, -y, -z'
' -x, -y, z'
' -x, y, -z'
' -x, y, z'
' x, -y, -z'
' x, -y, z'
' x, y, -z'
' x, y, z'
' -x+1/2, -y+1/2, -z+1/2'
' -x+1/2, -y+1/2, z+1/2'
' -x+1/2, y+1/2, -z+1/2'
' -x+1/2, y+1/2, z+1/2'
' x+1/2, -y+1/2, -z+1/2'
' x+1/2, -y+1/2, z+1/2'
' x+1/2, y+1/2, -z+1/2'
' x+1/2, y+1/2, z+1/2'

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_B_iso_or_equiv
Zr1 Zr   0 0 0.09509(43) 1 0.80(24)
O1 O   0 0 0.1026(29) 0.0473(14) 1 0.80(66)
O2 O   0 0.1493(37) 0 -0.0465(16) 1 0.80(66)
Zr2 Zr   0 0.15111(89) 0.10628(57) 0 1 0.80(24)
O3 O   0 0.1161(27) 0.2336(27) 0 1 0.80(66)
O4 O   0 0.3480(40) 0.0809(14) 0 1 0.80(66)
O5 O   0 0.2078(13) 0.15107(91) 0.07189(56) 1 0.80(66)
O6 O   0 0.1105(15) 0.0851(11) 0.13729(74) 1 0.80(66)
C1 C   0 0.1754275 0.1349718 0.1177686 1 0.80(90)
C2 C   0 0.2191206 0.1829315 0.1620391 1 0.80(90)
C3 C   0 0.2979756 0.2418603 0.1534018 1 0.80(90)
C4 C   0 0.3336952 0.2890573 0.1947299 1 0.80(90)
C5 C   0 0.2906671 0.2787477 0.2455273 1 0.80(90)
N6 N   0 0.1762682 0.1728096 0.2134025 0.5 0.80(90)
C6 C   0 0.1762682 0.1728096 0.2134025 0.5 0.80(90)
G1 O   0 0 0.5 0.5978(25) 1.000(71) 2.2(15)
G2 O   0 0.514(18) 0.1117(35) 0.6510(16) 0.500(25) 2.2(15)
G3 O   0 0 0.5 0.3110(23) 1.000(64) 2.2(15)
G4 O   0 0.5562(59) 0.1790(40) 0.4109(20) 0.500(30) 2.2(15)
G5 O   0 0 0.3220(62) 0.4431(35) 0.465(50) 2.2(15)

References: