Rhodamine functionalized mesoporous silica as chemosensor for efficient sensing of Al$^{3+}$, Cr$^{3+}$ and Fe$^{3+}$ ions and their removal from aqueous medium

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**Fig. s1** FT-IR spectra of (a) SBA-15, (b) APTES functionalized SBA-15, (c) TFMS, (d) RFMS and (e) Al-bound RFMS.

**Fig. s2** $^{29}$Si MAS NMR spectra of TFMS and RFMS.
Fig. s3 $^{13}$C CP MAS NMR spectra of TFMS and RFMS.

Fig. s4 Thermogravimetric analysis of (a) SBA-15, (b) 3-APTES loaded SBA-15, (c) TFMS and (d) RFMS.
**Fig. s5** UV-vis spectra of RFMS (0.05 g/L) in absence and in the presence of different metal ions (120 μM) in water/ethanol (14:1, v/v) at room temperature.

**Fig. s6** Plot of absorbance of RFMS (at 530 nm) versus concentration of Al$^{3+}$ ion.
**Fig. s7** Plot of absorbance of RFMS (at 530 nm) versus concentration of Cr$^{3+}$ ion.

**Fig. s8** Plot of absorbance of RFMS (at 530 nm) versus concentration of Fe$^{3+}$ ion.
**Fig. s9** Fluorescence spectra of RFMS (0.05 g/L) in absence and in the presence of different metal ions (120 μM) in water/ethanol (14:1, v/v) at room temperature.

**Fig. s10** Plot of fluorescence intensity of RFMS (at 550 nm) versus concentration of Al$^{3+}$ ion.
**Fig. s11** Plot of fluorescence intensity of RFMS (at 550 nm) versus concentration of Cr$^{3+}$ ion.

**Fig. s12** Plot of fluorescence intensity of RFMS (at 550 nm) versus concentration of Fe$^{3+}$ ion.
**Determination of LOD of RFMS:**

Limit of detection (LOD) for our probe has been determined by $3\sigma$ method by the following equation: $DL = K \times Sb1/S$. Where $K = 2$ or $3$ (3 in this case); here $Sb1$ is the standard deviation of the blank solution (Fig. s13); and $S$ is the slope of the calibration curve obtained from Linear dynamic plot of F.I. vs $[M^{3+}]$ µM (Fig. s14, s15 and s16).

Here $Sb1 = 949.1195$, $S = 526941.52$ (for $Al^{3+}$), $310077.16$ (for $Cr^{3+}$) and $3939.36$ (for $Fe^{3+}$).

- LOD of $Al^{3+} = (3 \times 949.1195)/(541803.820) = 5.40$ nM
- LOD of $Cr^{3+} = (3 \times 949.1195)/(448979.334) = 9.18$ nM
- LOD of $Fe^{3+} = (3 \times 949.1195)/(4566.881) = 722.80$ nM

*Fig. s13* Determination of $Sb1$ of the blank, RFMS in solution.
Fig. s14 Linear dynamic plot of F.I. (at 550 nm) vs. [Al\(^{3+}\)] for the determination of S (slope).

Fig. s15 Linear dynamic plot of F.I. (at 550 nm) vs. [Cr\(^{3+}\)] for the determination of S (slope).
Fig. s16 Linear dynamic plot of F.I. (at 550 nm) vs. [Fe$^{3+}$] for the determination of S (slope).

Fig. s17 Excited state fluorescence decay behavior of RFMS and its complexes Al$^{3+}$, Cr$^{3+}$ and Fe$^{3+}$ ions in ethanol/water mixture (1:14, v/v) at room temperature.
Determination of various cations adsorbed on RFMS by Titrmetric Method

Strength of the stock solutions:

- Zn-acetate = 1.002 (M/100)
- Lead nitrate = 1.001 (M/100)
- Potassium dichromate = 1.004 (N/100)
- Na₂EDTA = 1.005 (M/100)

Determination of Fe³⁺
Estimated by direct titration with potassium dichromate solution.
Volume of Potassium dichromate solution need for 25 mL of iron solution = 23.7 mL
Volume of Potassium dichromate solution need for 25 mL of iron solution treated with 0.10 g of RFMS = 15.4 mL
Therefore in 25 mL of iron solution Fe³⁺ present = 0.01328 g
After treating with RFMS in 25 ml of iron solution Fe³⁺ present = 0.00863 g
Amount of Fe³⁺ adsorbed by 0.10 g of RFMS = 0.00465 g

Determination of Zn²⁺
Estimated by direct titration with Na₂EDTA solution.
Volume of Na₂EDTA solution need for 25 mL of zinc solution = 23.1 mL
Volume of Na₂EDTA solution need for 25 mL of zinc solution treated with 0.10 g of RFMS = 22 mL
Therefore in 25 mL of zinc solution, Zn²⁺ present = 0.01517 g
After treating with 0.10 g of RFMS in 25 mL of zinc solution, Zn²⁺ present = 0.01445 g
Amount of Zn²⁺ adsorbed by 0.10 g of RFMS = 0.00072 g

Determination of Pb²⁺
Estimated by back titration of excess Na₂EDTA with zinc acetate solution. (25 mL metal ion + 50 mL Na₂EDTA solution)
Volume of zinc acetate solution need for 25 mL of Pb²⁺ solution = 25.6 mL
Volume of zinc acetate solution need for 25 mL of Pb²⁺ solution treated with 0.10 g of RFMS = 26.2 mL
Therefore in 25 mL of lead solution Pb\(^{2+}\) present = 0.050333 g
After treating with 0.10 g of RFMS in 25 mL of lead solution Pb\(^{2+}\) present= 0.049827 g
Amount of Pb\(^{2+}\) adsorbed by 0.10 g of RFMS = 0.000503 g

For mixture also 0.10 g of RFMS is taken in every case

**Determination of Pb\(^{2+}\) and Fe\(^{3+}\) in a mixture**
Iron adsorbed =0.0034 g
Lead adsorbed = 0.00221 g

**Determination of Zn\(^{2+}\) and Fe\(^{3+}\) in a mixture**
Iron adsorbed =0.00425 g
Zincadsorbed = 0.00121 g
Table S1 Comparison of some parameters of some recently published related research works

<table>
<thead>
<tr>
<th>SI No.</th>
<th>Probe</th>
<th>Metal ion analyzed</th>
<th>Excitation (nm)/Emission (nm)</th>
<th>Fluorescence intensity enhancement</th>
<th>LOD (M)</th>
<th>Linearity range</th>
<th>Application</th>
<th>Removal efficiency</th>
<th>Maximum uptake capacity</th>
<th>Ref</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td><img src="image1" alt="Probe" /></td>
<td>Al&lt;sup&gt;3+&lt;/sup&gt;, Cr&lt;sup&gt;3+&lt;/sup&gt;, and Fe&lt;sup&gt;3+&lt;/sup&gt;</td>
<td>Colorimetric detection (color change: colorless to yellow); absorption band at 425 nm</td>
<td>2.16 × 10&lt;sup&gt;−6&lt;/sup&gt; (Al&lt;sup&gt;3+&lt;/sup&gt;), 1.27 × 10&lt;sup&gt;−8&lt;/sup&gt; (Cr&lt;sup&gt;3+&lt;/sup&gt;) and 5.03 × 10&lt;sup&gt;−9&lt;/sup&gt; (Fe&lt;sup&gt;3+&lt;/sup&gt;)</td>
<td>0 to 30 μl (Al&lt;sup&gt;3+&lt;/sup&gt;), 0 to 60 μl (Cr&lt;sup&gt;3+&lt;/sup&gt;) and 0 to 60 μl (Fe&lt;sup&gt;3+&lt;/sup&gt;)</td>
<td>Logic gate</td>
<td>--</td>
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<td>2</td>
<td><img src="image2" alt="Probe" /></td>
<td>Al&lt;sup&gt;3+&lt;/sup&gt;, Cr&lt;sup&gt;3+&lt;/sup&gt;, and Fe&lt;sup&gt;3+&lt;/sup&gt;</td>
<td>480/583</td>
<td>--</td>
<td>0.22 × 10&lt;sup&gt;−6&lt;/sup&gt; (Al&lt;sup&gt;3+&lt;/sup&gt;), 0.63 × 10&lt;sup&gt;−6&lt;/sup&gt; (Cr&lt;sup&gt;3+&lt;/sup&gt;) and 0.14 × 10&lt;sup&gt;−6&lt;/sup&gt; (Fe&lt;sup&gt;3+&lt;/sup&gt;)</td>
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<td>3</td>
<td><img src="image3" alt="Probe" /></td>
<td>Al&lt;sup&gt;3+&lt;/sup&gt;, Cr&lt;sup&gt;3+&lt;/sup&gt;, and Fe&lt;sup&gt;3+&lt;/sup&gt;</td>
<td>502/558</td>
<td>31 (Al) 26 (Cr) 41 (Fe)</td>
<td>1.34 × 10&lt;sup&gt;−6&lt;/sup&gt; (Al&lt;sup&gt;3+&lt;/sup&gt;), 2.28 × 10&lt;sup&gt;−6&lt;/sup&gt; (Cr&lt;sup&gt;3+&lt;/sup&gt;) and 1.28 × 10&lt;sup&gt;−6&lt;/sup&gt; (Fe&lt;sup&gt;3+&lt;/sup&gt;)</td>
<td>Not mentioned</td>
<td>(i) Logic gate (ii) Cell imaging</td>
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<td>Al&lt;sup&gt;3+&lt;/sup&gt;, Cr&lt;sup&gt;3+&lt;/sup&gt;, and Fe&lt;sup&gt;3+&lt;/sup&gt;</td>
<td>500/552</td>
<td>98 (Al) 50 (Cr) 38 (Fe)</td>
<td>1.18 × 10&lt;sup&gt;−9&lt;/sup&gt; (Al&lt;sup&gt;3+&lt;/sup&gt;), 1.80 × 10&lt;sup&gt;−9&lt;/sup&gt; (Cr&lt;sup&gt;3+&lt;/sup&gt;) and 4.04 × 10&lt;sup&gt;−9&lt;/sup&gt; (Fe&lt;sup&gt;3+&lt;/sup&gt;)</td>
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<td>Logic gate</td>
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<td><img src="image5" alt="Probe" /></td>
<td>Al&lt;sup&gt;3+&lt;/sup&gt;, Cr&lt;sup&gt;3+&lt;/sup&gt;, and Fe&lt;sup&gt;3+&lt;/sup&gt;</td>
<td>Colorimetric detection (color change: colorless to light yellow); absorption band at ~420 nm</td>
<td>2.8 × 10&lt;sup&gt;−7&lt;/sup&gt; (Al&lt;sup&gt;3+&lt;/sup&gt;), 2.5 × 10&lt;sup&gt;−7&lt;/sup&gt; (Cr&lt;sup&gt;3+&lt;/sup&gt;) and 1.10 × 10&lt;sup&gt;−7&lt;/sup&gt; (Fe&lt;sup&gt;3+&lt;/sup&gt;)</td>
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<td>Zn&lt;sup&gt;2+&lt;/sup&gt;</td>
<td>360/509</td>
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<td>1.08 × 10&lt;sup&gt;−7&lt;/sup&gt;</td>
<td>0–6 μM</td>
<td>Removal of metal ion</td>
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<td>157.2 mg/g (adsorption capacity)</td>
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<td>No.</td>
<td>Structure</td>
<td>Metal Ion</td>
<td>Molecular Weight</td>
<td>pH</td>
<td>Stock Concentration</td>
<td>Removal of Metal Ion</td>
<td>Analysis Technique</td>
<td>Recovery</td>
<td>Adsorption Capacity</td>
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<td><img src="image" alt="Al³⁺" /></td>
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<td>325/427</td>
<td>8.5</td>
<td>Not mentioned</td>
<td>87.4%</td>
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<td>0.1 × 10⁻⁹</td>
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<td>27a</td>
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<td>1.5 × 10⁻⁸</td>
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<td>27b</td>
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<td>Hg²⁺</td>
<td>530/589</td>
<td>--</td>
<td>9.05 × 10⁻⁷</td>
<td>(i) Removal of metal ion (ii) cell imaging</td>
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<td>115.47 mg/g (adsorption capacity)</td>
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<td><img src="image" alt="RFMS" /></td>
<td>Al³⁺, Cr³⁺, and Fe³⁺</td>
<td>500/550</td>
<td>145 (Al) 174 (Cr) 30 (Fe)</td>
<td>23.5 × 10⁻⁹ (Al³⁺), 13.4 × 10⁻⁹ (Cr³⁺) and 69.7 × 10⁻⁹ (Fe³⁺)</td>
<td>Removal of metal ion</td>
<td>97.28 (Al) 97.06 (Cr) 96.87 (Fe)</td>
<td>11.20 (Al), 19.72 (Cr) and 21.55 (Fe) mg/g</td>
<td>Present study</td>
<td></td>
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</table>

*** Stock solution of the metal ion is 1× 10⁻³ M