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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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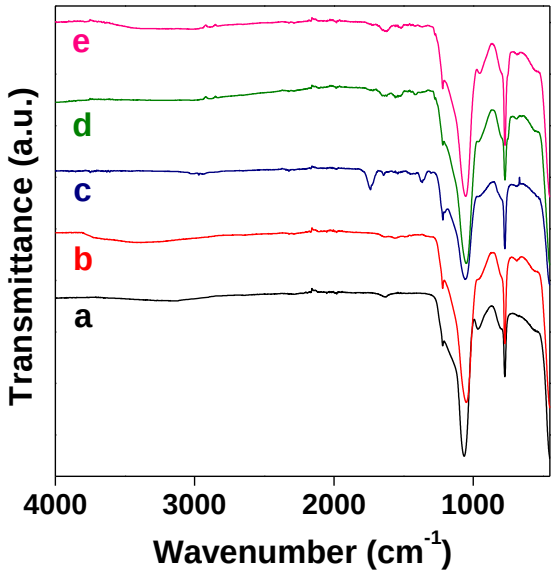


Fig. s1 FT-IR spectra of (a) SBA-15, (b) APTES functionalized SBA-15, (c) **TFMS**, (d) **RFMS** and (e) Al-bound **RFMS**.

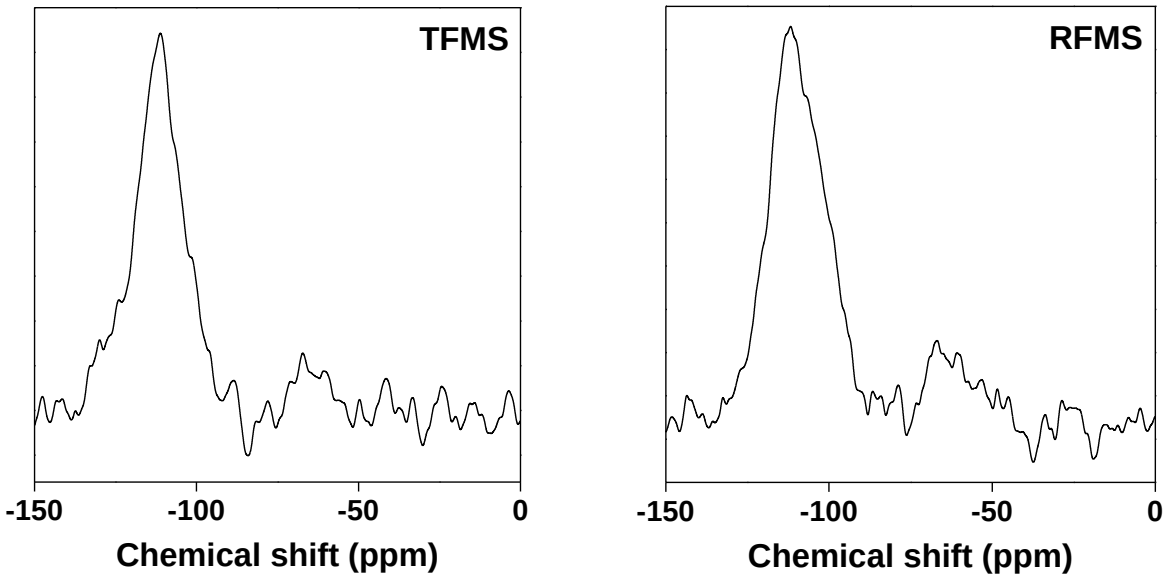


Fig. s2 ^{29}Si MAS NMR spectra of **TFMS** and **RFMS**.

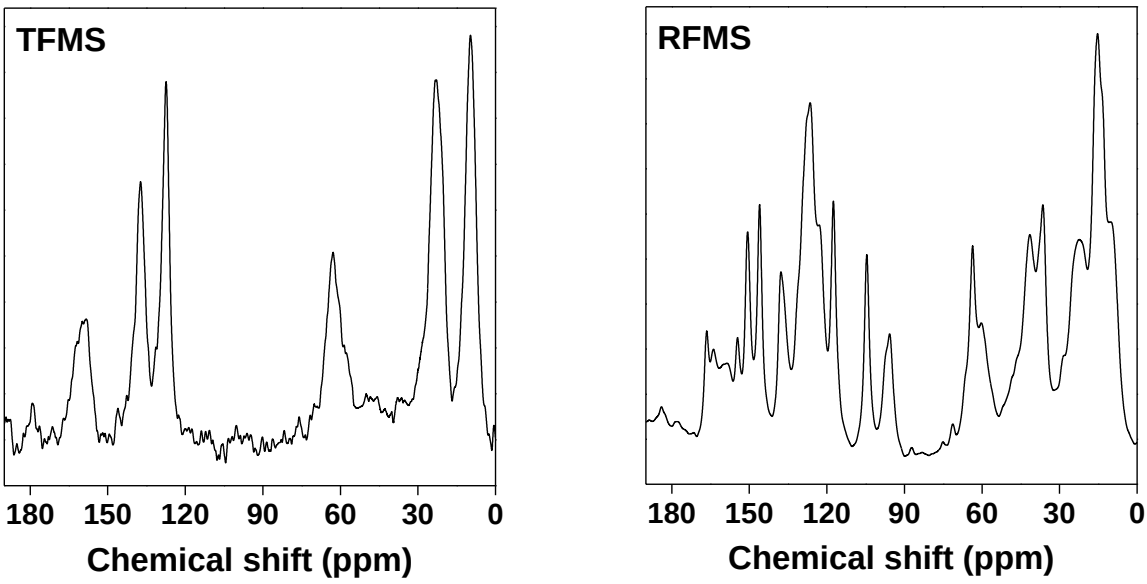


Fig. s3 ^{13}C CP MAS NMR spectra of **TFMS** and **RFMS**.

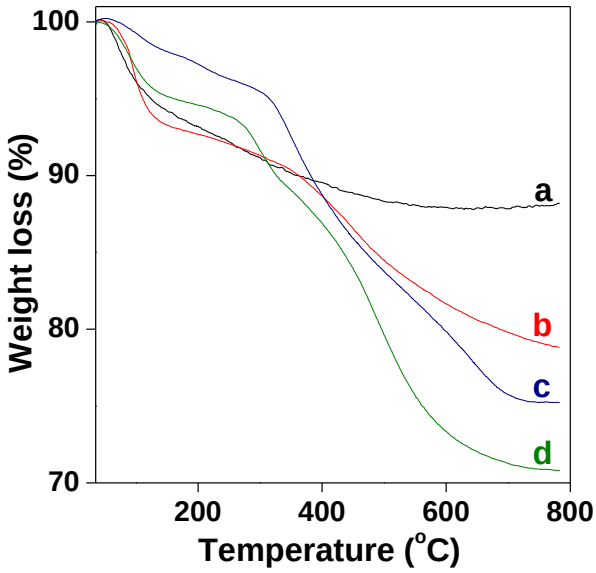


Fig. s4 Thermogravimetric analysis of (a) SBA-15, (b) 3-APTES loaded SBA-15, (c) **TFMS** and (d) **RFMS**.

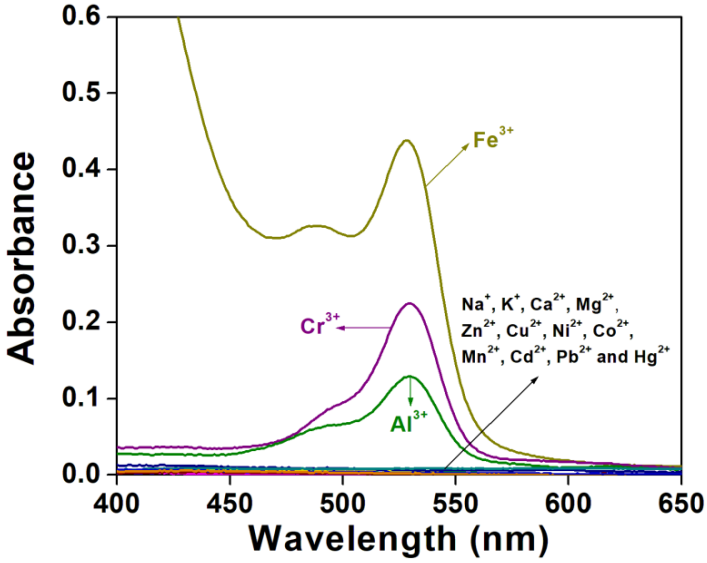


Fig. s5 UV-vis spectra of **RFMS** (0.05 g/L) in absence and in the presence of different metal ions (120 μM) in water/ethanol (14:1, v/v) at room temperature.

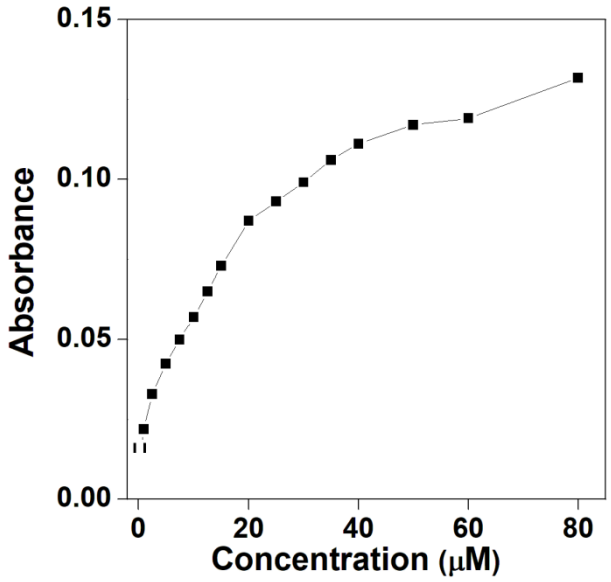


Fig. s6 Plot of absorbance of **RFMS** (at 530 nm) versus concentration of Al^{3+} ion.

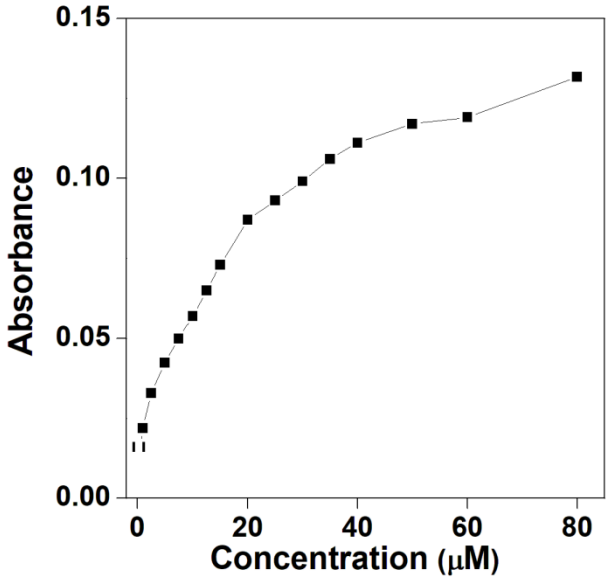


Fig. s7 Plot of absorbance of **RFMS** (at 530 nm) versus concentration of Cr^{3+} ion.

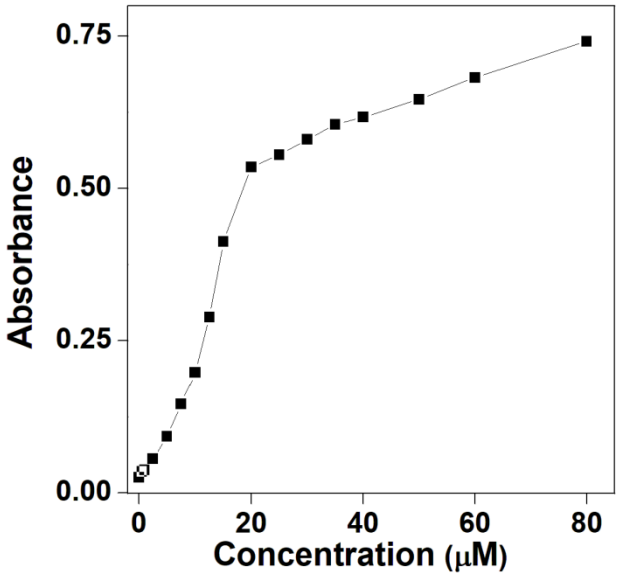


Fig. s8 Plot of absorbance of **RFMS** (at 530 nm) versus concentration of Fe^{3+} ion.

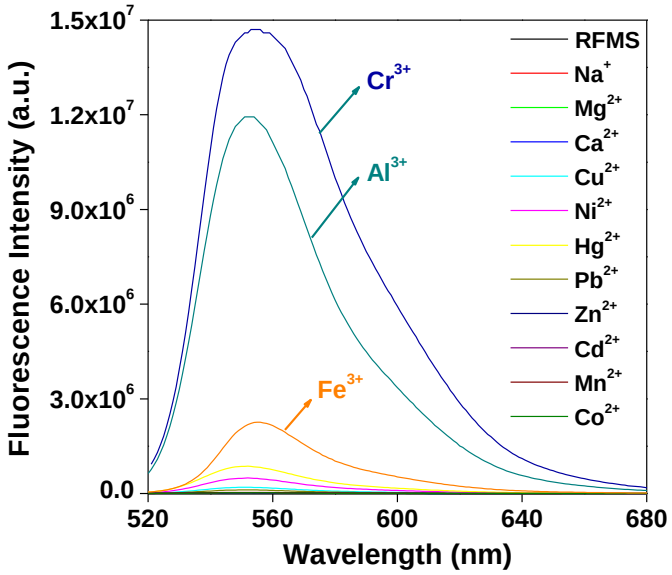


Fig. s9 Fluorescence spectra of **RFMS** (0.05 g/L) in absence and in the presence of different metal ions (120 μM) in water/ethanol (14:1, v/v) at room temperature.

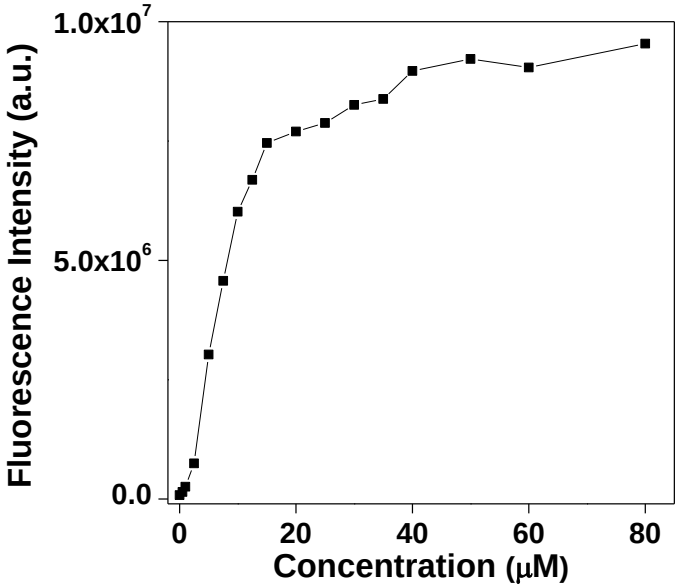


Fig. s10 Plot of fluorescence intensity of **RFMS** (at 550 nm) versus concentration of Al^{3+} ion.

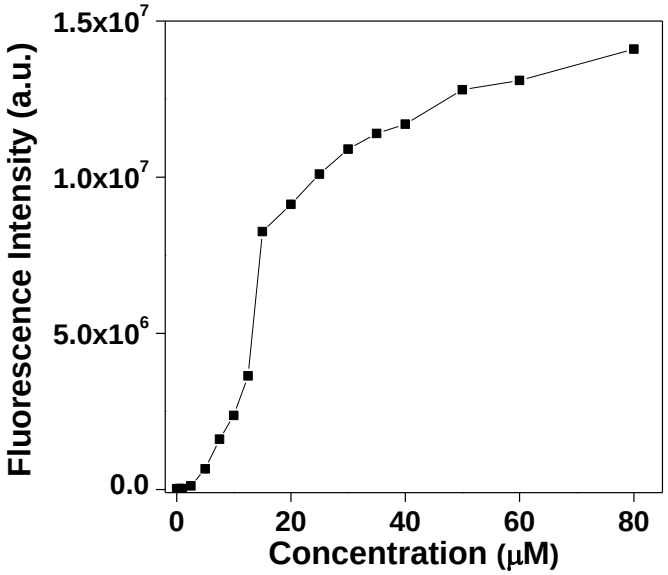


Fig. s11 Plot of fluorescence intensity of **RFMS** (at 550 nm) versus concentration of Cr^{3+} ion.

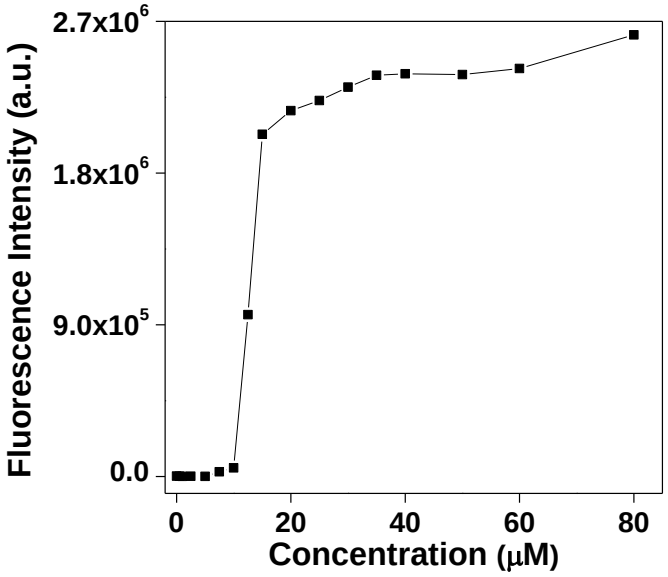


Fig. s12 Plot of fluorescence intensity of **RFMS** (at 550 nm) versus concentration of Fe^{3+} ion.

Determination of LOD of RFMS:

Limit of detection (LOD) for our probe has been determined by 3σ method by the following equation: DL = K* 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 × 949.1195)/ (541803.820) = 5.40 nM

LOD of Cr^{3+} = (3 × 949.1195)/ (448979.334) = 9.18 nM

LOD of Fe^{3+} = (3 × 949.1195)/ (4566.881) = 722.80 nM

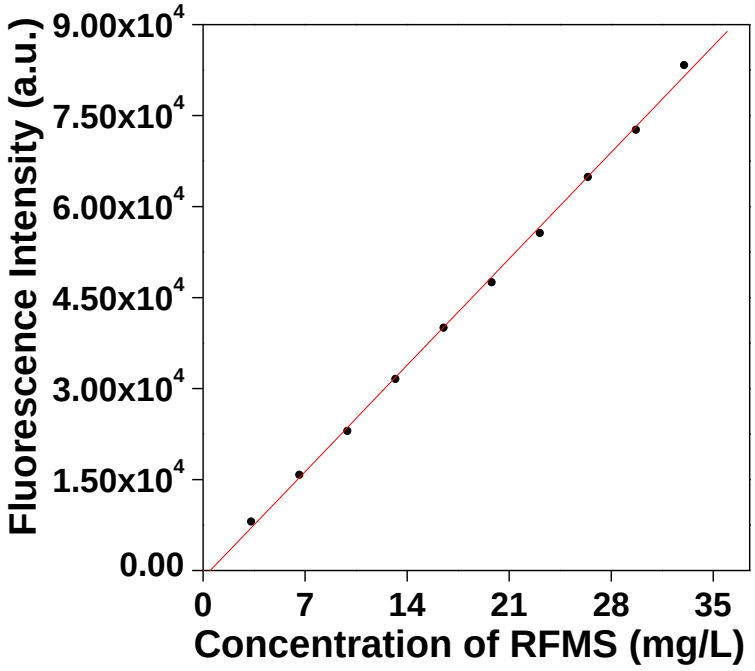


Fig. s13 Determination of Sb1 of the blank, **RFMS** in solution.

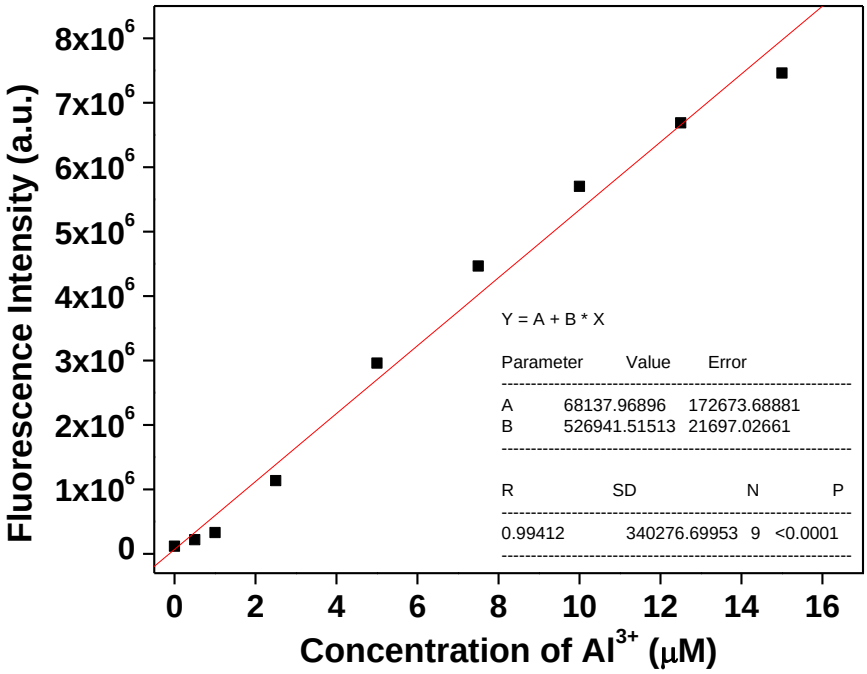


Fig. s14 Linear dynamic plot of F.I. (at 550 nm) vs. [Al^{3+}] for the determination of S (slope).

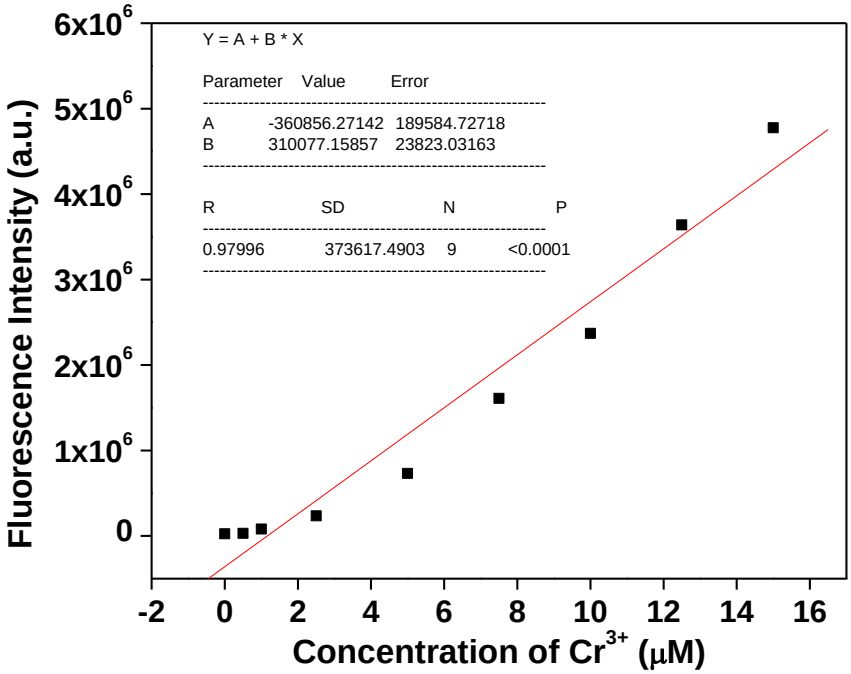


Fig. s15 Linear dynamic plot of F.I. (at 550 nm) vs. [Cr^{3+}] for the determination of S (slope).

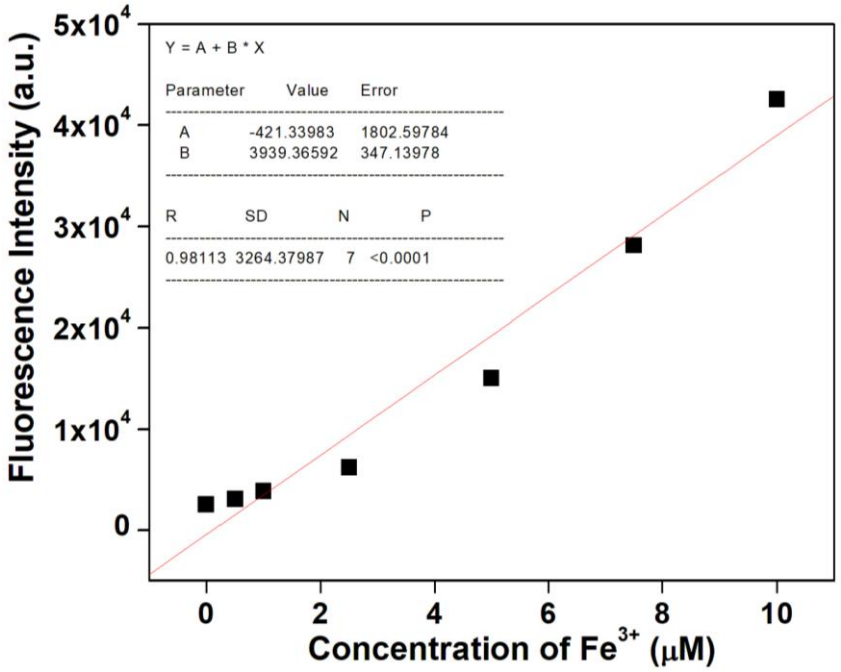


Fig. s16 Linear dynamic plot of F.I. (at 550 nm) vs. [Fe^{3+}] for the determination of S (slope).

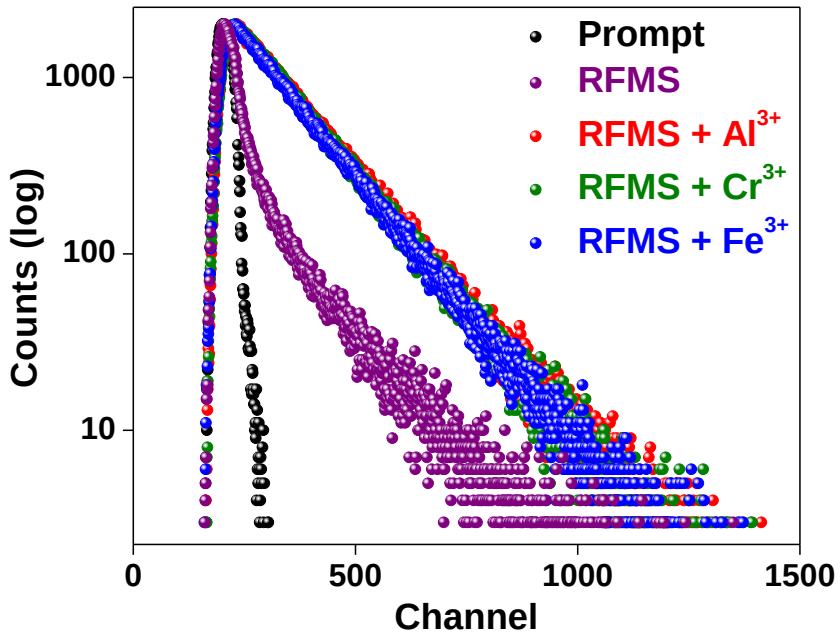


Fig. s17 Excited state fluorescence decay behavior of **RFMS** and and its complexes Al^{3+}, Cr^{3+} and Fe^{3+} ions in ethanol/water mixture (1:14, v/v) at room temperature.

Determination of various cations adsorbed on RFMS by Titrimetric Method

Strength of the stock solutions:

- Zn-acetate =1.002 (M/100)
- Lead nitrate=1.001 (M/100)
- Potassium dichromate=1.004 (N/100)
- Na_2EDTA = 1.005 (M/100)

Determination of Fe^{3+}

Estimated by direct titration with potassium dichromate solution.

Volume of Potassium dichromate solution need for 25 mLof iron solution = 23.7mL

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 Fe^{3+} present = 0.01328g

After treating with **RFMS** in 25 ml of iron solution Fe^{3+} present = 0.00863 g

Amount of Fe^{3+} adsorbed by 0.10 g of **RFMS** = 0.00465 g

Determination of Zn^{2+}

Estimated by direct titration with Na_2EDTA solution.

Volume of Na_2EDTA solution need for 25 mL of zinc solution =23.1 mL

Volume of Na_2EDTA solution need for 25 mLof zinc solution treated with 0.10 g of RFMS =22 mL

Therefore in 25 ml of zinc solution, Zn^{2+} present = 0.01517 g

After treating with 0.10 g of **RFMS** in 25 mLof zinc solution, Zn^{2+} present = 0.01445 g

Amount of Zn^{2+} adsorbed by 0.10 g of **RFMS** =0.00072 g

Determination of Pb^{2+}

Estimated by back titration of excess Na_2EDTA with zinc acetate solution. (25 mL metal ion + 50mLNa_2EDTA solution)

Volume of zinc acetate solution need for 25 mL of Pb^{2+} solution = 25.6 mL

Volume of zinc acetate solution need for 25 mL of Pb^{2+}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

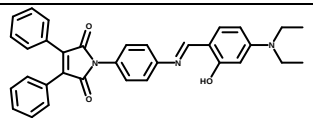
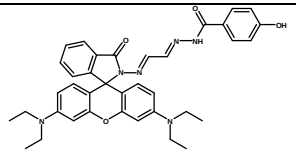
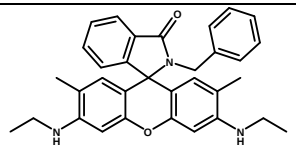
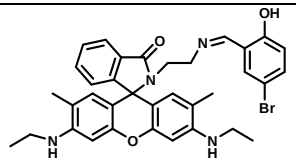
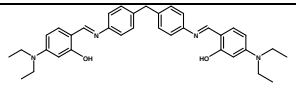
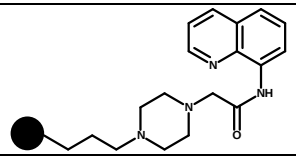
Lead adsorbed = 0.00221 g

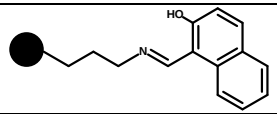
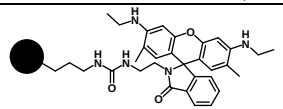
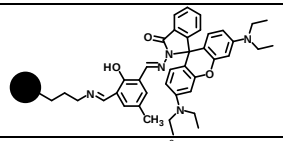
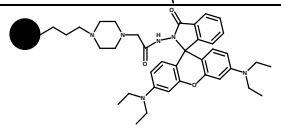
Determination of Zn^{2+} and Fe^{3+}in a mixture

Iron adsorbed =0.00425 g

Zincadsorbed = 0.00121 g

Table S1 Comparison of some parameters of some recently published related research works

Sl No.	Probe	Metal ion analyzed	Excitation (nm)/ Emission (nm)	Fluorescence intensity enhancement	LOD (M)	Linearity range	Application	Removal efficiency	Maximum uptake capacity	Ref
1		Al^{3+}, Cr^{3+} and Fe^{3+}	Colorimetric detection (color change: colorless to yellow); absorption band at 425 nm		2.16×10^{-6} (Al^{3+}), 1.27×10^{-8} (Cr^{3+}) and 5.03×10^{-8} (Fe^{3+})	0 to 30 µl (Al^{3+}), 0 to 60 µl (Cr^{3+}) and 0 to 60 µl (Fe^{3+})***	Logic gate	---		20
2		Al^{3+}, Cr^{3+} and Fe^{3+}	480/583	--	0.22×10^{-6} (Al^{3+}), 0.63×10^{-6} (Cr^{3+}) and 0.14×10^{-6} (Fe^{3+})	Not mentioned	No	--	--	21
3		Al^{3+}, Cr^{3+} and Fe^{3+}	502/558	31 (Al) 26 (Cr) 41 (Fe)	1.34×10^{-6} (Al^{3+}), 2.28×10^{-6} (Cr^{3+}) and 1.28×10^{-6} (Fe^{3+})	Not mentioned	(i) Logic gate (ii) Cell imaging	--	--	22
4		Al^{3+}, Cr^{3+} and Fe^{3+}	500/552	98 (Al) 50 (Cr) 38 (Fe)	1.18×10^{-9} (Al^{3+}), 1.80×10^{-9} (Cr^{3+}) and 4.04×10^{-9} (Fe^{3+})	Not mentioned	Logic gate	--	--	23
5		Al^{3+}, Cr^{3+} and Fe^{3+}	Colorimetric detection (color change: colorless to light yellow); absorption band at ~420 nm		2.8×10^{-7} (Al^{3+}), 2.5×10^{-7} (Cr^{3+}) and $1.\times 10^{-7}$ (Fe^{3+})	Not mentioned	Logic gate	---		40
6		Zn^{2+}	360/509	--	1.08×10^{-7}	0–6 µM	Removal of metal ion	--	157.2 mg/g (adsorption capacity)	25a

7		Al^{3+}	325/427	8.5	17.84×10^{-6}	Not mentioned	Removal of metal ion	87.4%	--	26
8		Hg^{2+}	497/552	--	0.1×10^{-9}	1.0–100.0 nM	Analysis of metal ion in real sample	109.5% recovery	--	27a
9		Hg^{2+}	500/580	--	1.5×10^{-8}	Not mentioned	Logic gate	--	--	27b
10		Hg^{2+}	530/589	--	9.05×10^{-7}	0–6 × 10^{-5} M	(i) Removal of metal ion (ii) cell imaging	--	115.47 mg/g (adsorption capacity)	28
11	**RFMS**	Al^{3+}, Cr^{3+} and Fe^{3+}	500/550	145 (Al) 174 (Cr) 30 (Fe)	23.5×10^{-9} (Al^{3+}), 13.4×10^{-9} (Cr^{3+}) and 69.7×10^{-9} (Fe^{3+})	0-15 μM (Al^{3+}), 2.5-12.5 μM (Cr^{3+}) and 0-10 μM (Fe^{3+})	Removal of metal ion	97.28 (Al) 97.06 (Cr) 96.87 (Fe)	11.20 (Al), 19.72 (Cr) and 21.55 (Fe) mg/g	Present study

*** Stock solution of the metal ion is 1×10^{-3} M