

Selective Dye Sorption and Metal Ions Sensing Behaviours of a New Cd-based MOF

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ELECTRONIC SUPPLEMENTARY INFORMATION

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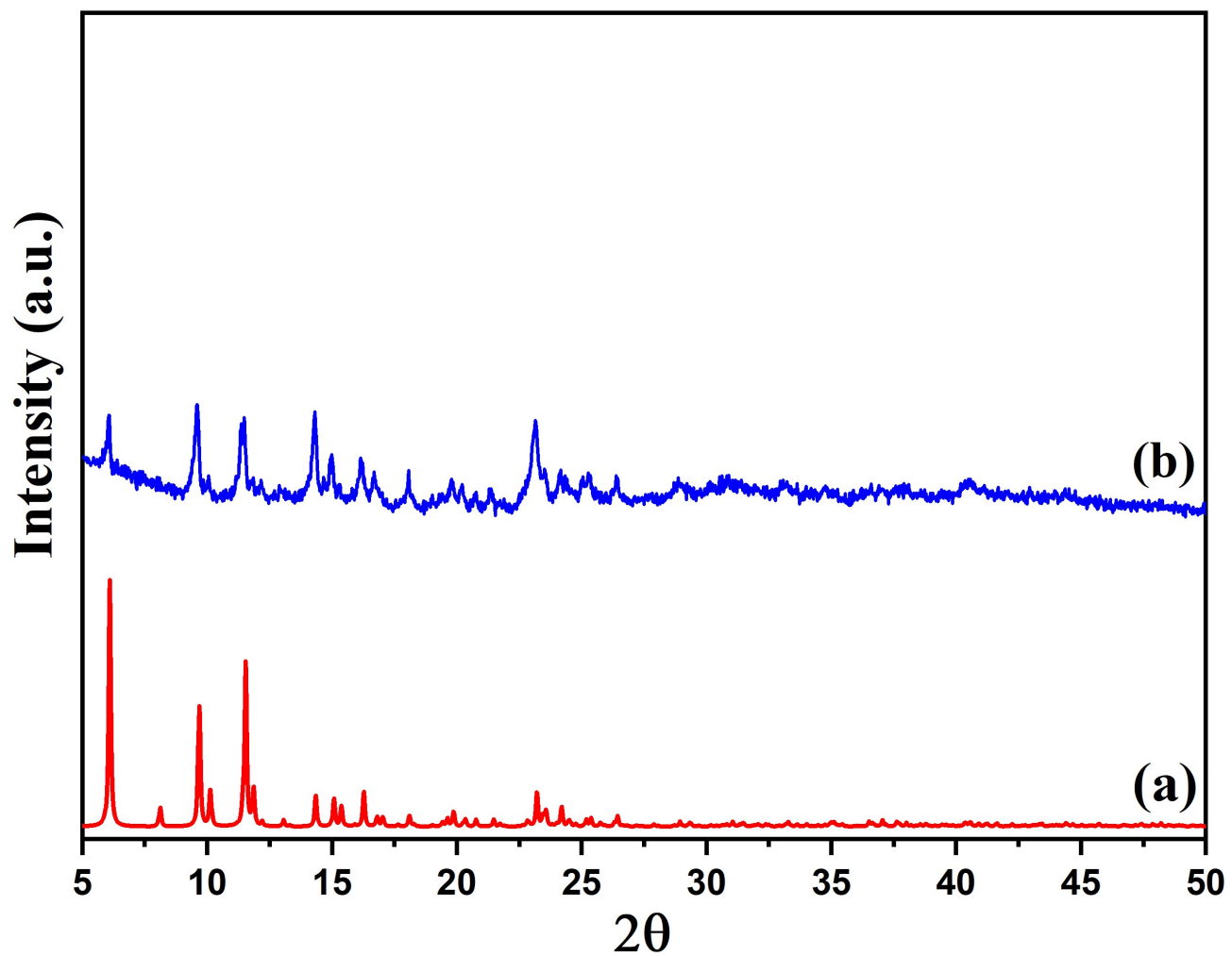


Fig. S1: Powder XRD (CuK α) patterns of [Cd(PDA)(L)₂], **1**: (a) simulated from single crystal X-ray data, (b) experimental.

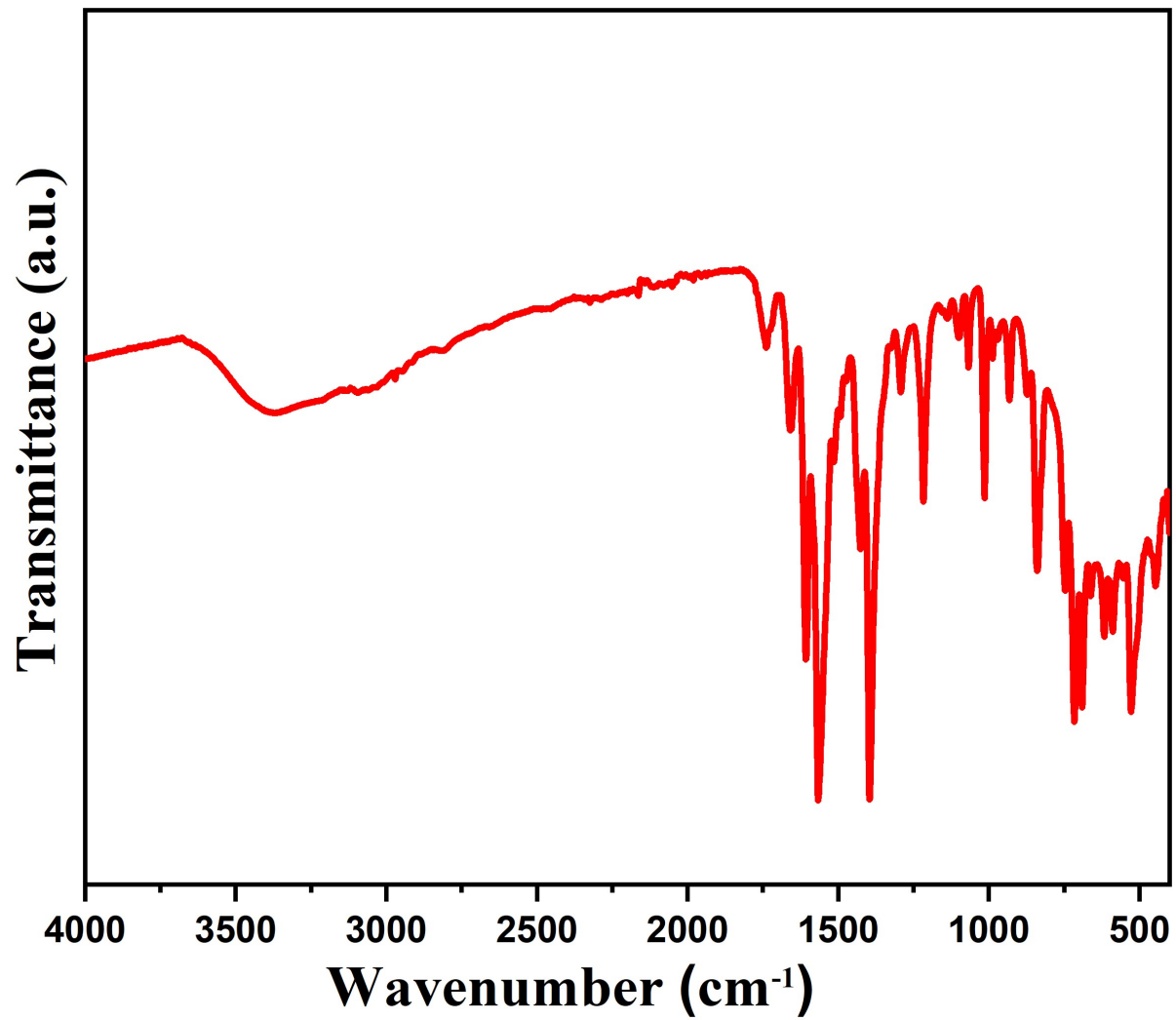


Fig. S2: IR spectrum of $[\text{Cd}(\text{PDA})(\text{L})_2]$, 1.

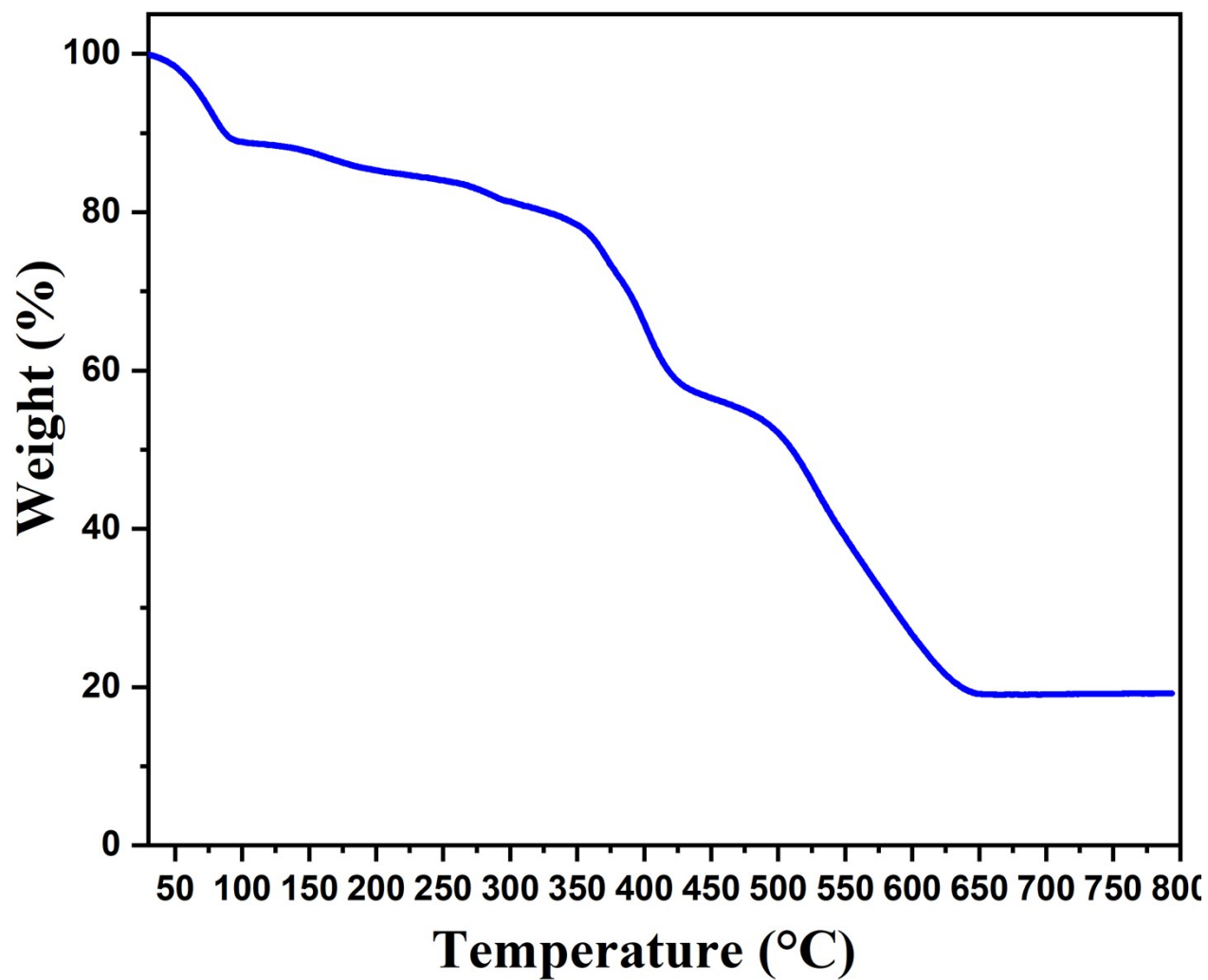


Fig. S3: Thermogravimetric analysis (TGA) of [Cd(PDA)(L)₂], **1**, in nitrogen atmosphere.

Table S1: Selected Bond Angles (deg) observed in [Cd(PDA)(L)₂], **1**.

Angle	Amplitude (°)
O (1) –Cd(1)–O(1) # 1	83.9 (3)
O (1) –Cd(1)–N(3) # 2	91.35 (17)
O (1) # 1 –Cd(1)–N(3) # 2	91.36 (17)
O (1) –Cd(1)–N(1)	91.57 (16)
O (1) # 1–Cd(1)–N(1)	91.57 (16)
N (3) # 2–Cd(1)–N(1)	176.1 (2)
O (1) –Cd(1)–N(2)	137.93 (13)
O (1) # 1–Cd(1)–N(2)	137.93 (13)
N (3) # 2–Cd(1)–N(2)	91.3 (3)
N (1) –Cd(1)–N(2)	84.7 (2)
O (1) –Cd(1)–O(2)	53.85 (17)
O (1) # 1–Cd(1)–O(2)	137.72 (18)
N (3) # 2–Cd(1)–O(2)	91.91 (13)
N (1) –Cd(1)–O(2)	87.70 (13)
N (2) –Cd(1)–O(2)	84.10 (11)
O (1) –Cd(1)–O(2) # 1	137.72 (17)
O (1) # 1 –Cd(1)–O(2) # 1	53.85 (17)
N (3) # 2 –Cd(1)–O(2) # 1	91.91 (13)
N (1) –Cd(1)–O(2)	87.70 (13)
N (2) –Cd(1)–O(2)	84.10 (11)
O (1) –Cd(1)–O(2) # 1	137.72 (17)
O (1) # 1 –Cd(1)–O(2) # 1	53.85 (17)
N (3) # 2 –Cd(1)–O(2) # 1	91.91 (13)
N (1) –Cd(1)–O(2) # 1	87.70 (13)
N (2) –Cd(1)–O(2) # 1	84.10 (12)
O (2) –Cd(1)–O(2) # 1	167.7 (2)

Symmetry transformations used to generate equivalent atoms:

For 1: #1 -x+1, y, z; #2 -x+1, -y+1, -z+1.

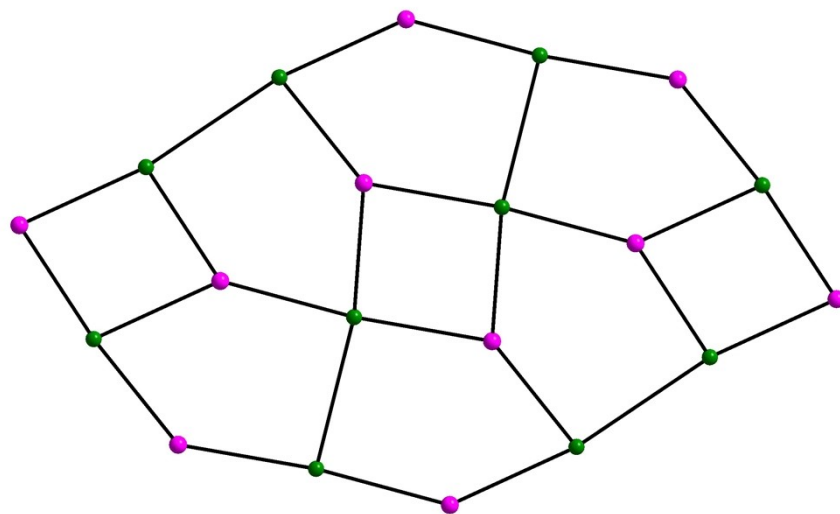


Fig. S4: Figure shows the network structure based on 3-connected L ligands and four connected Cd^{2+} ions of $[\text{Cd}(\text{PDA})(\text{L})_2]$, **1**.

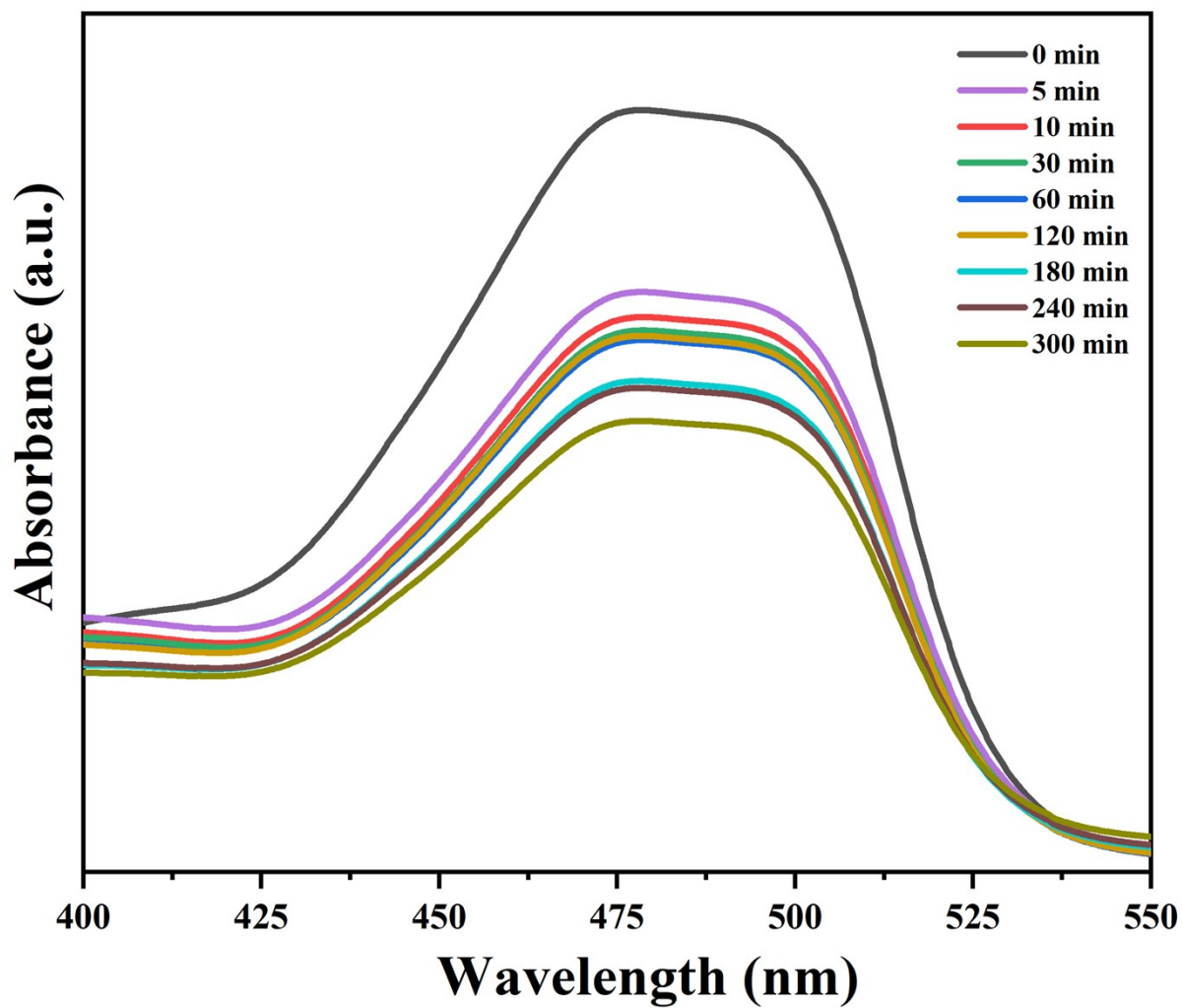


Fig. S5: UV-Vis absorption spectra of Orange G (OG) during the time dependent sorption study using compound 1.

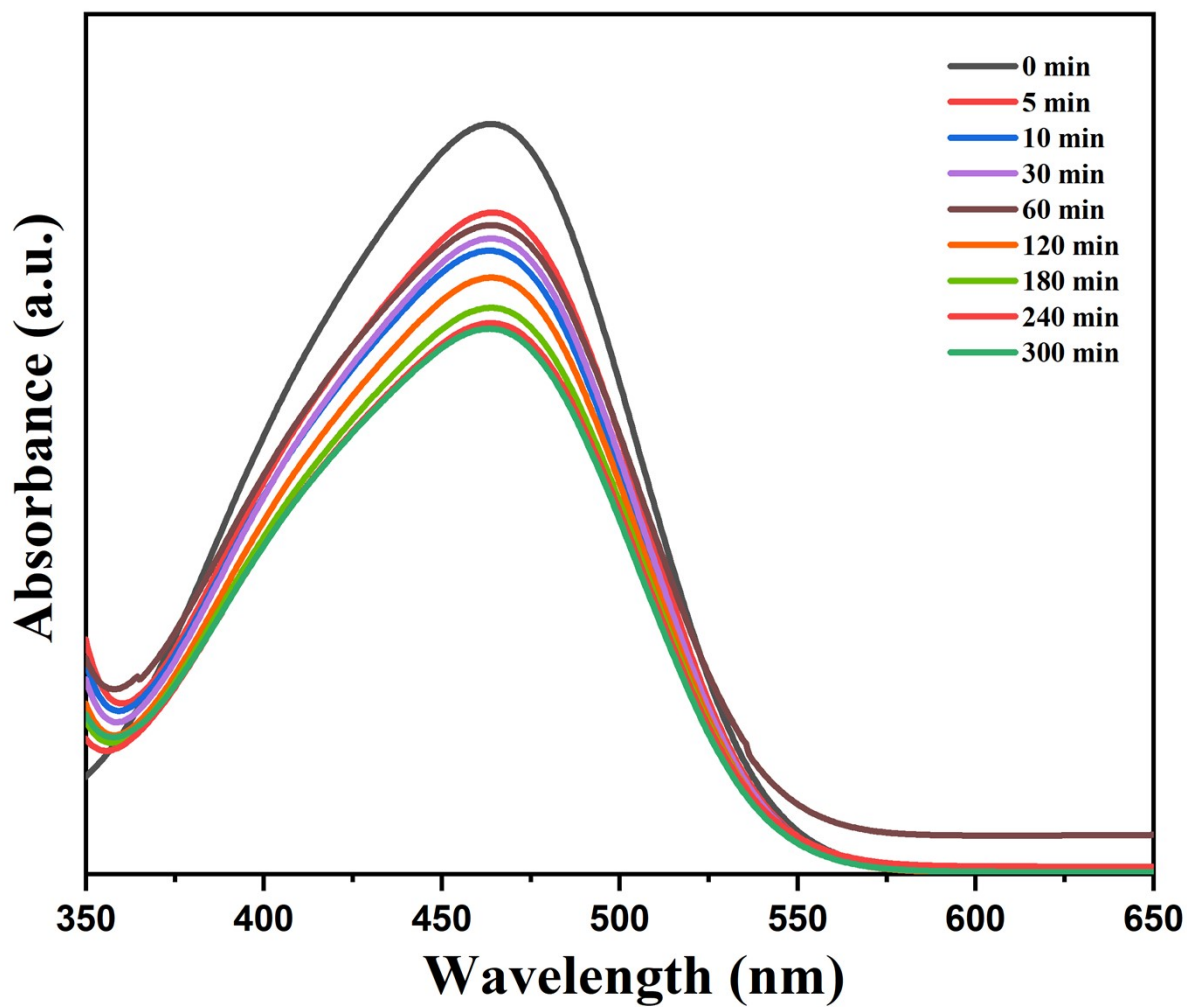


Fig. S6: UV-Vis absorption spectra of Methyl Orange (MO) during the time dependent sorption study using compound **1**.

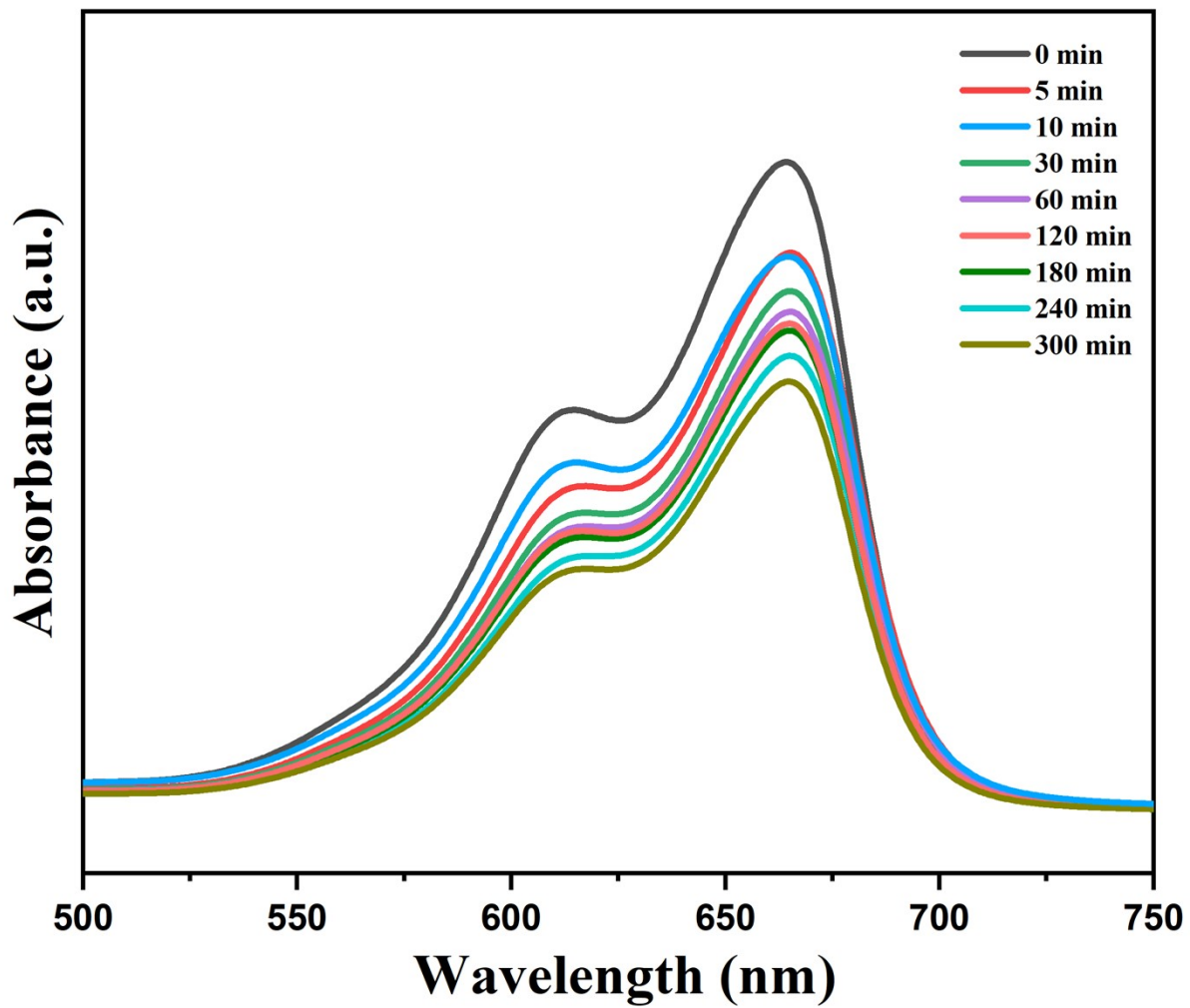


Fig. S7: UV-Vis absorption spectra of Methylene Blue (MB) during the time dependent sorption study using compound **1**.

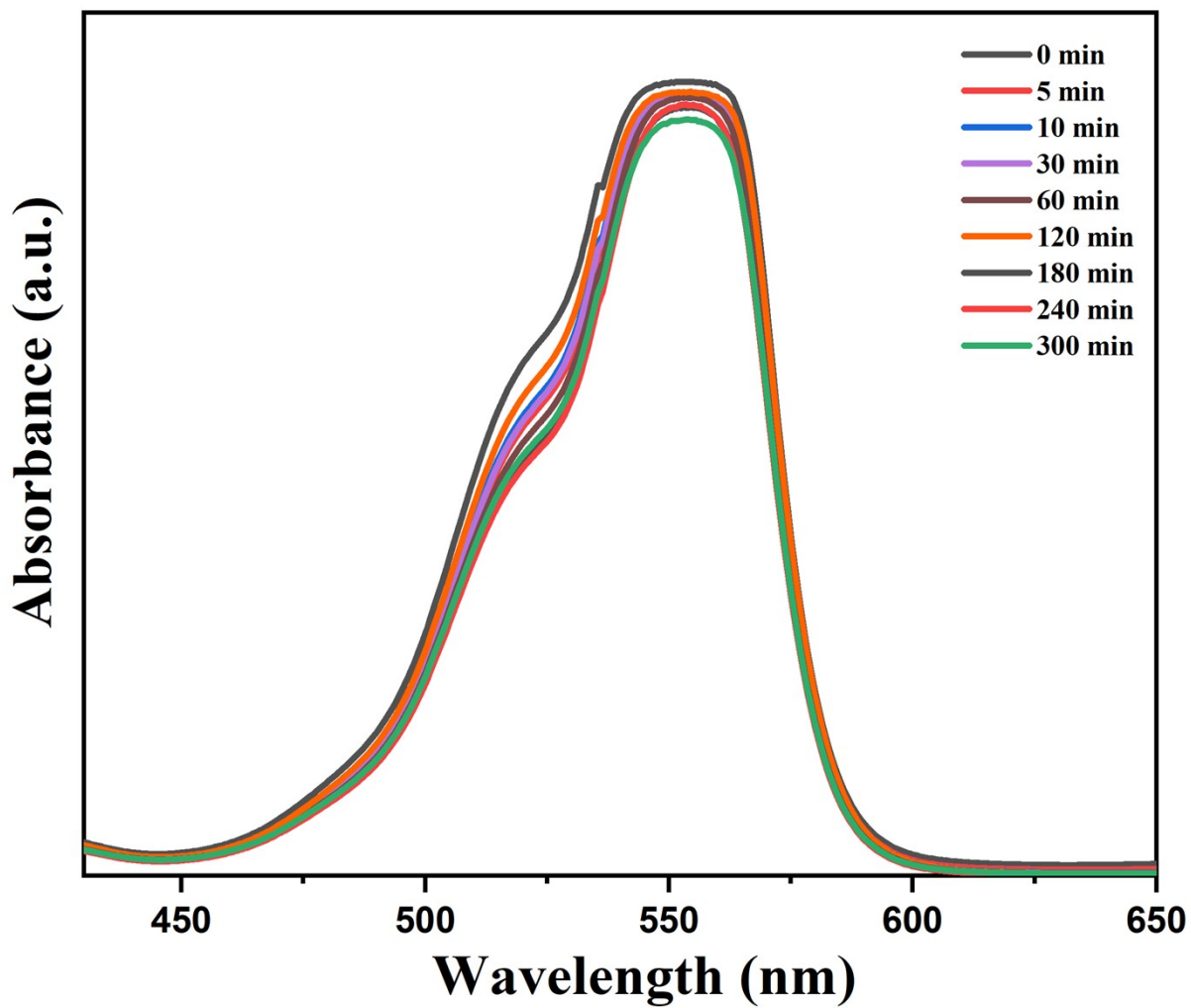


Fig. S8: UV-Vis absorption spectra of Rhodamine B (RhB) during the time dependent sorption study using compound **1**.

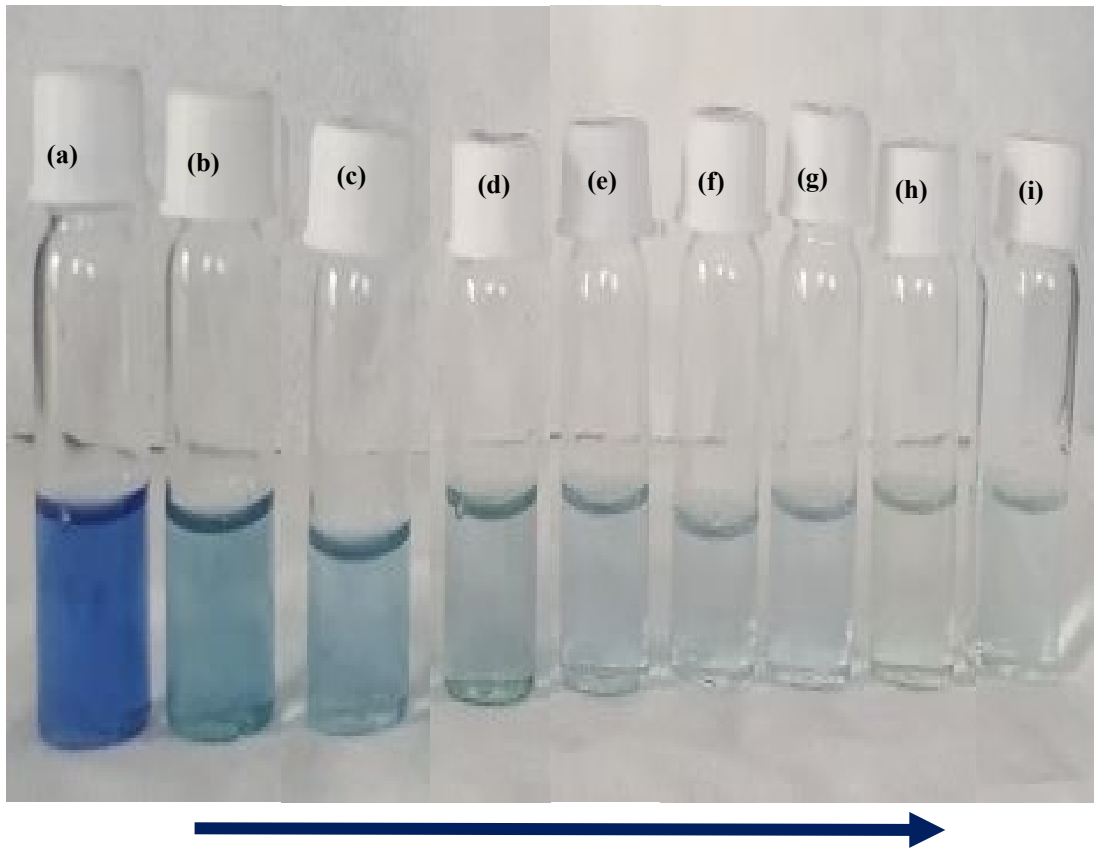


Fig. S9: Figure shows the photographs of colour intensity changes of the RBBR during the sorption study: (a) initial solution, (b) after 5 min, (c) after 10 min, (d) after 30 min, (e) after 60 min, (f) after 120 min, (h) after 180 min, (h) after 240 min, (i) after 300 min.

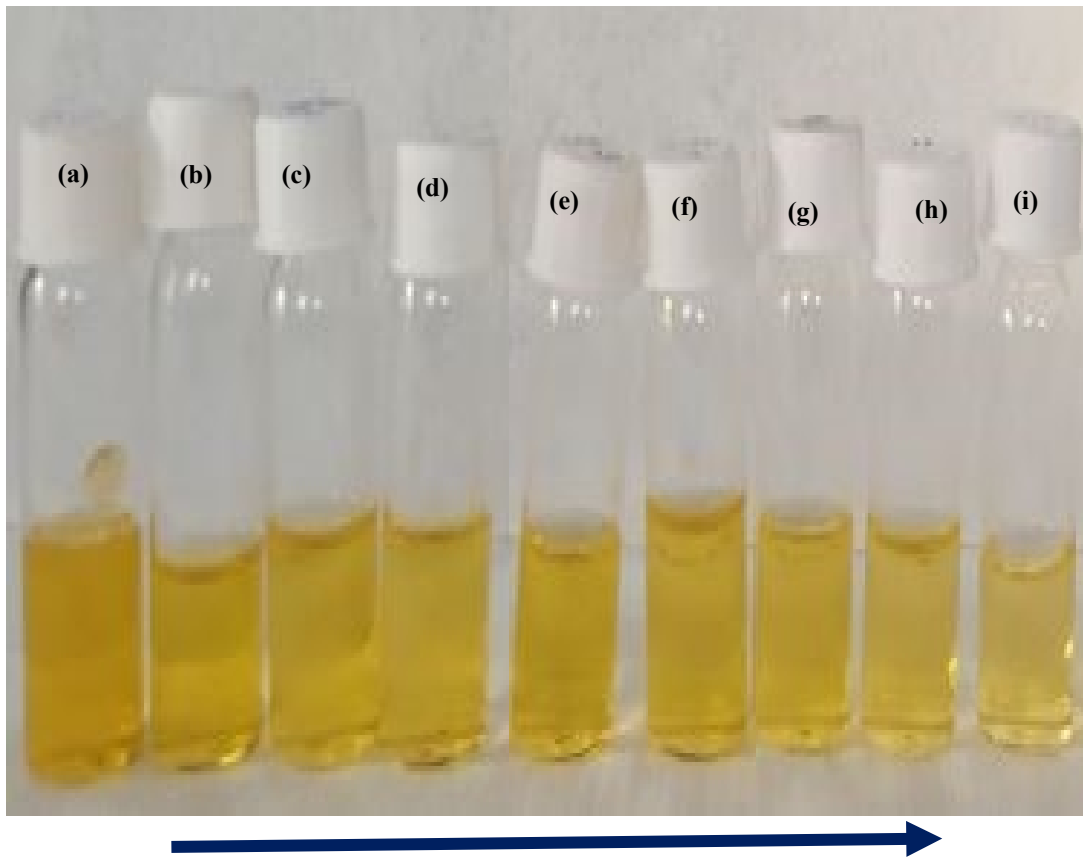


Fig. S10: Figure shows the photographs of colour intensity changes of the OG during the sorption study: (a) initial solution, (b) after 5 min, (c) after 10 min, (d) after 30 min, (e) after 60 min, (f) after 120 min, (h) after 180 min, (h) after 240 min, (i) after 300 min.

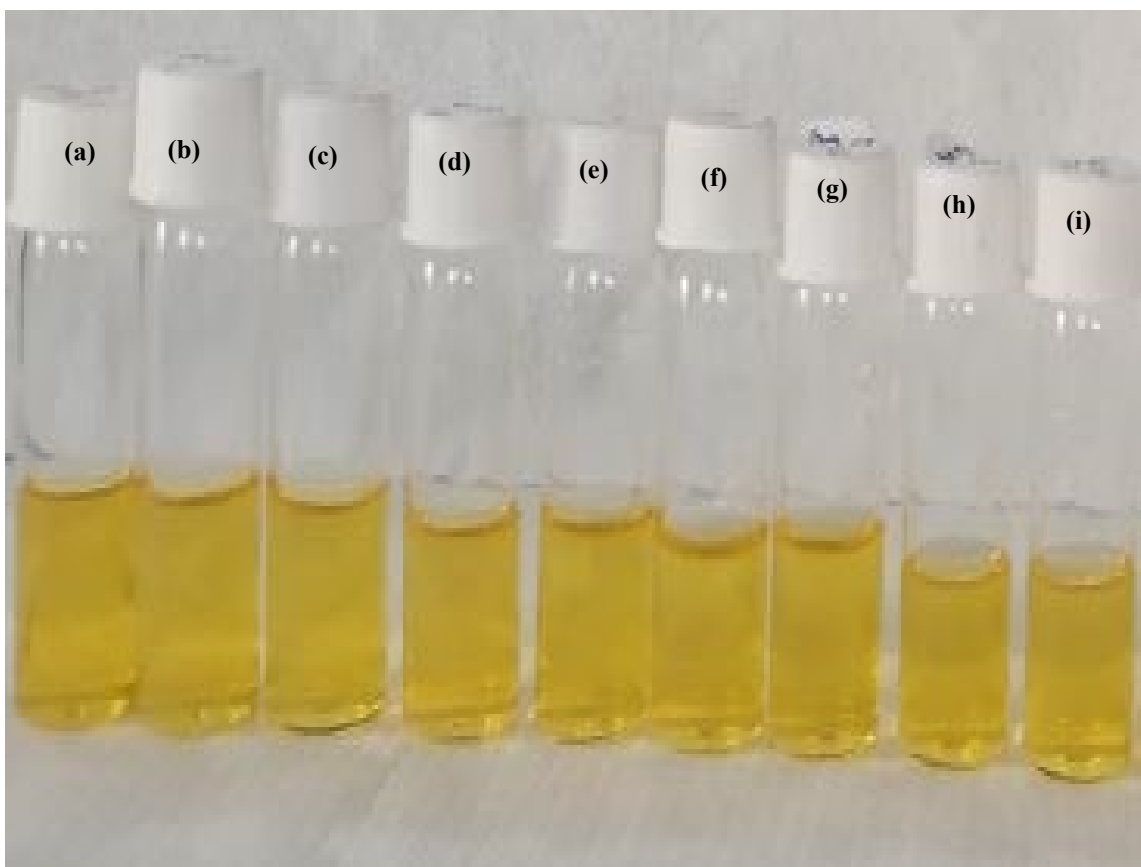


Fig. S11: Figure shows the photographs of colour intensity changes of the MO during the sorption study: (a) initial solution, (b) after 5 min, (c) after 10 min, (d) after 30 min, (e) after 60 min, (f) after 120 min, (h) after 180 min, (h) after 240 min, (i) after 300 min.

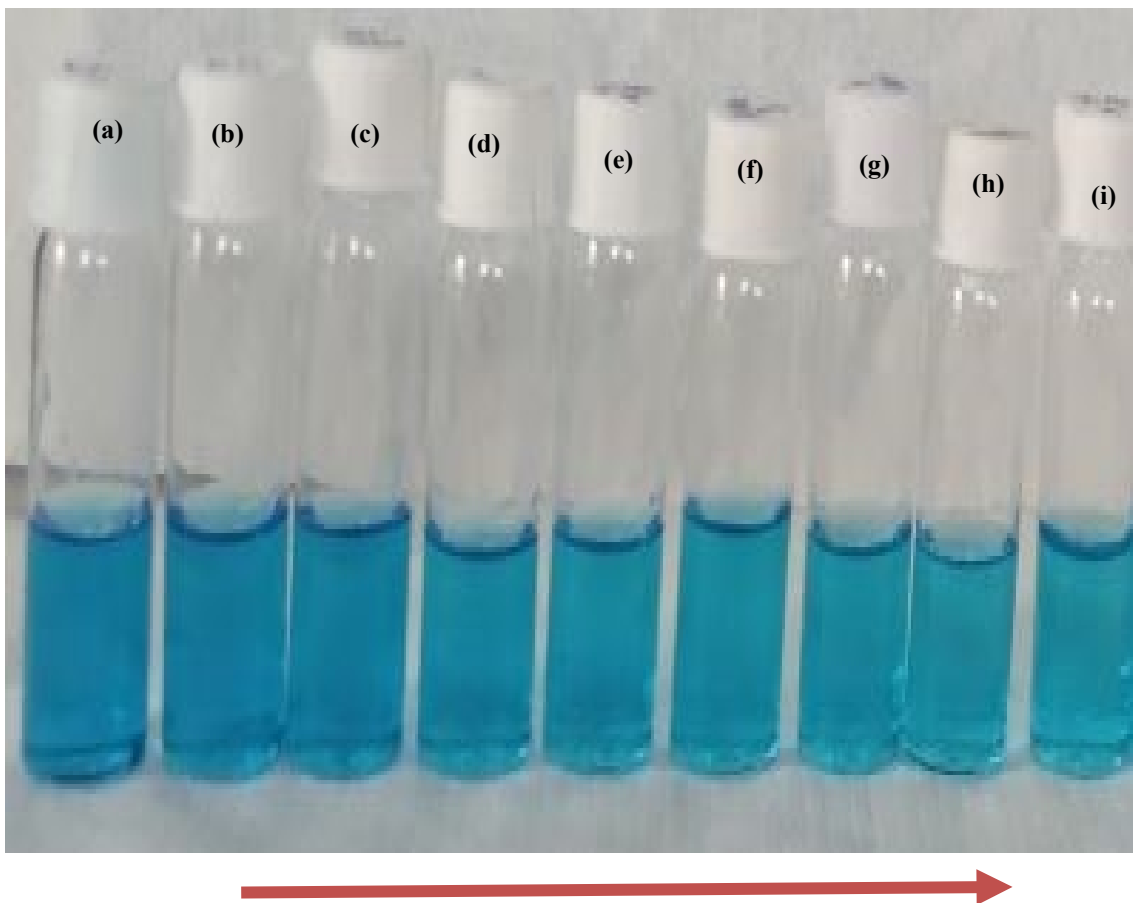


Fig. S12: Figure shows the photographs of colour intensity changes of the MB during the sorption study: (a) initial solution, (b) after 5 min, (c) after 10 min, (d) after 30 min, (e) after 60 min, (f) after 120 min, (h) after 180 min, (h) after 240 min, (i) after 300 min.

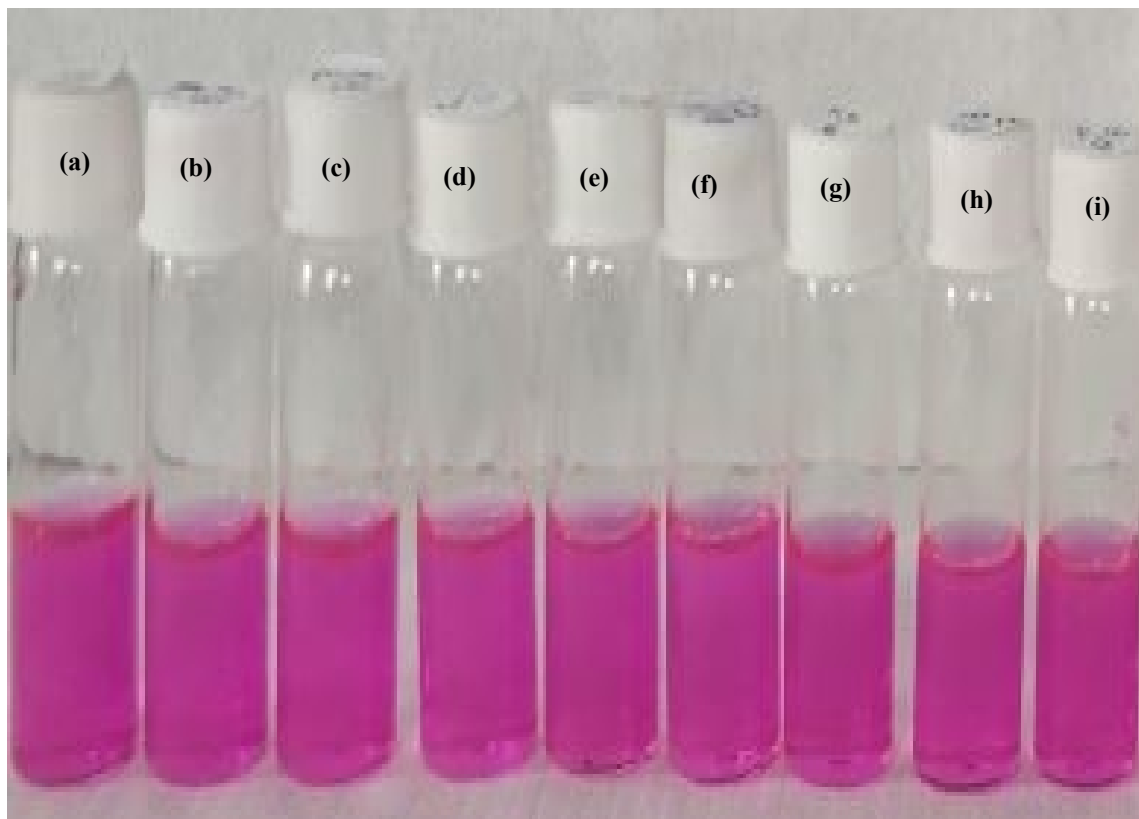


Fig.
S13:

Figure shows the photographs of colour intensity changes of the RhB during the sorption study: (a) initial solution, (b) after 5 min, (c) after 10 min, (d) after 30 min, (e) after 60 min, (f) after 120 min, (g) after 180 min, (h) after 240 min, (i) after 300 min.

Table S2: Pseudo-second-order kinetic parameters for RBBR dye sorption into $[\text{Cd}(\text{PDA})(\text{L})_2]$, 1.

Adsorbent	q_e (mg g ⁻¹)	K_2 (h g mg ⁻¹)	R^2
Cd-MOF	31.23	0.292	0.998
	61.50	0.112	0.996
	93.63	0.051	0.995
	123.15	0.056	0.997
	152.20	0.042	0.997

Table S3: Parameters of Langmuir model for RBBR dye sorption into [Cd(PDA)(L)₂], **1**.

Adsorbent	Dye	K_L (L mg ⁻¹)	Q_m (mg g ⁻¹)	R^2
Cd-MOF	RBBR	0.071	263.15	1

Table S4: A Summary of RBBR dye sorption using various materials.

Materials	Efficiency (%)	Time	Ref.
NMIL88(Fe)-Lac and HS NMIL88(Fe)-Lac	90.8 and 92.0	3 h and 2 h	79
ZIF-8 and ZIF-67	98 and 95	2 h	80
TiO ₂ -ZrO ₂ - Laccase and TiO ₂ - ZrO ₂ -SiO ₂ - Laccase	90 and 76	24 h	81
Magnetic copper alginate beads	75.8	4 h	82
CS-SA/ALG/MTN	54.3	½ h	83
Immobilized laccase	64	48 h	84
PU microspheres	64.1	6 h	85
Trametes maxima IIPLC-32	92.3	—	86
Amberlyst A21	89.23	2½ h	87
Thuja orientalis (ACTOL)	82	5 h	88
[Cd(PDA)(L) ₂]	95	5 h	This work

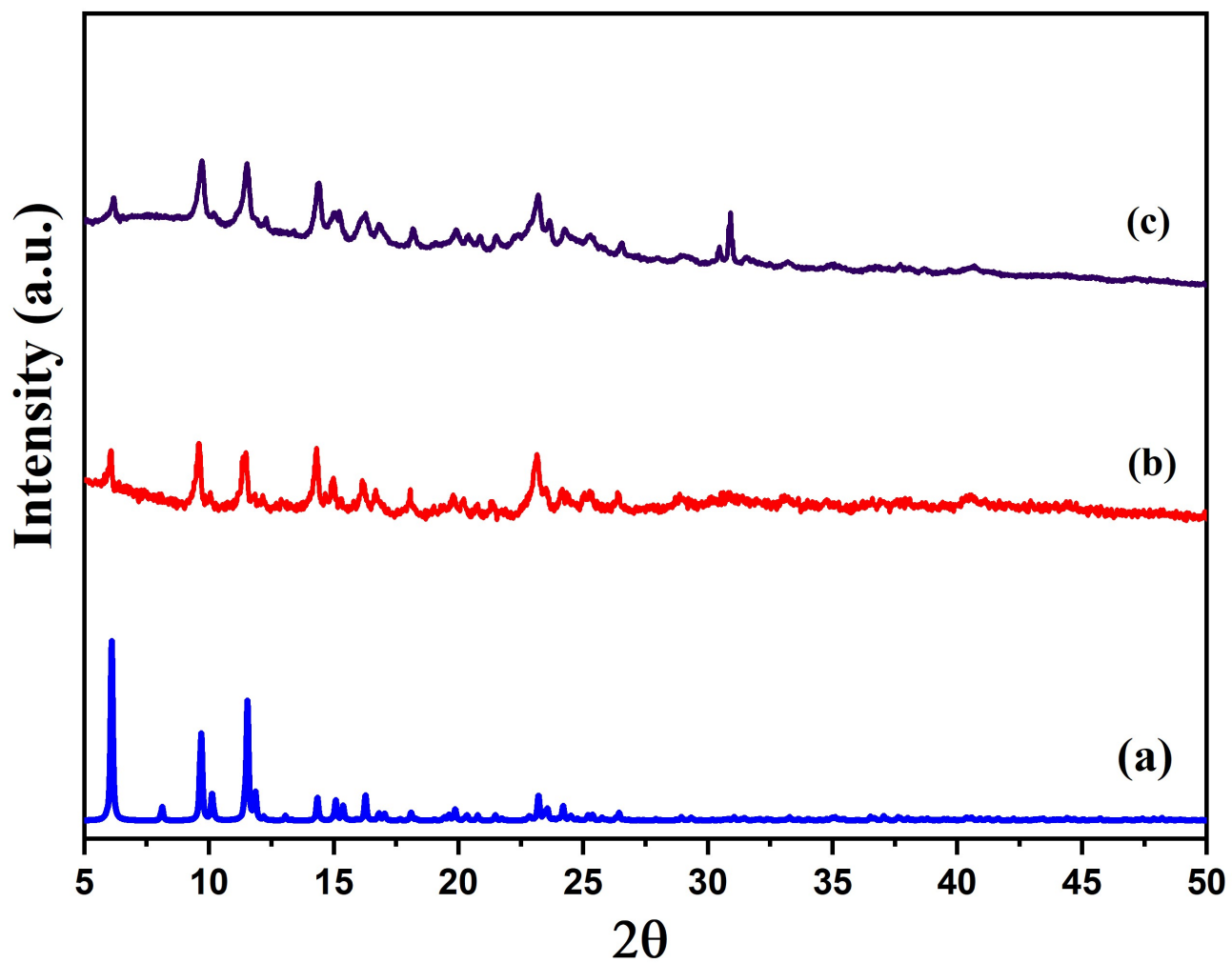


Fig. S14: Powder XRD (CuK α) patterns of [Cd(PDA)(L)₂], 1: (a) simulated from single crystal X-ray data, (b) experimental. (c) RBBR@1 after 300 min.

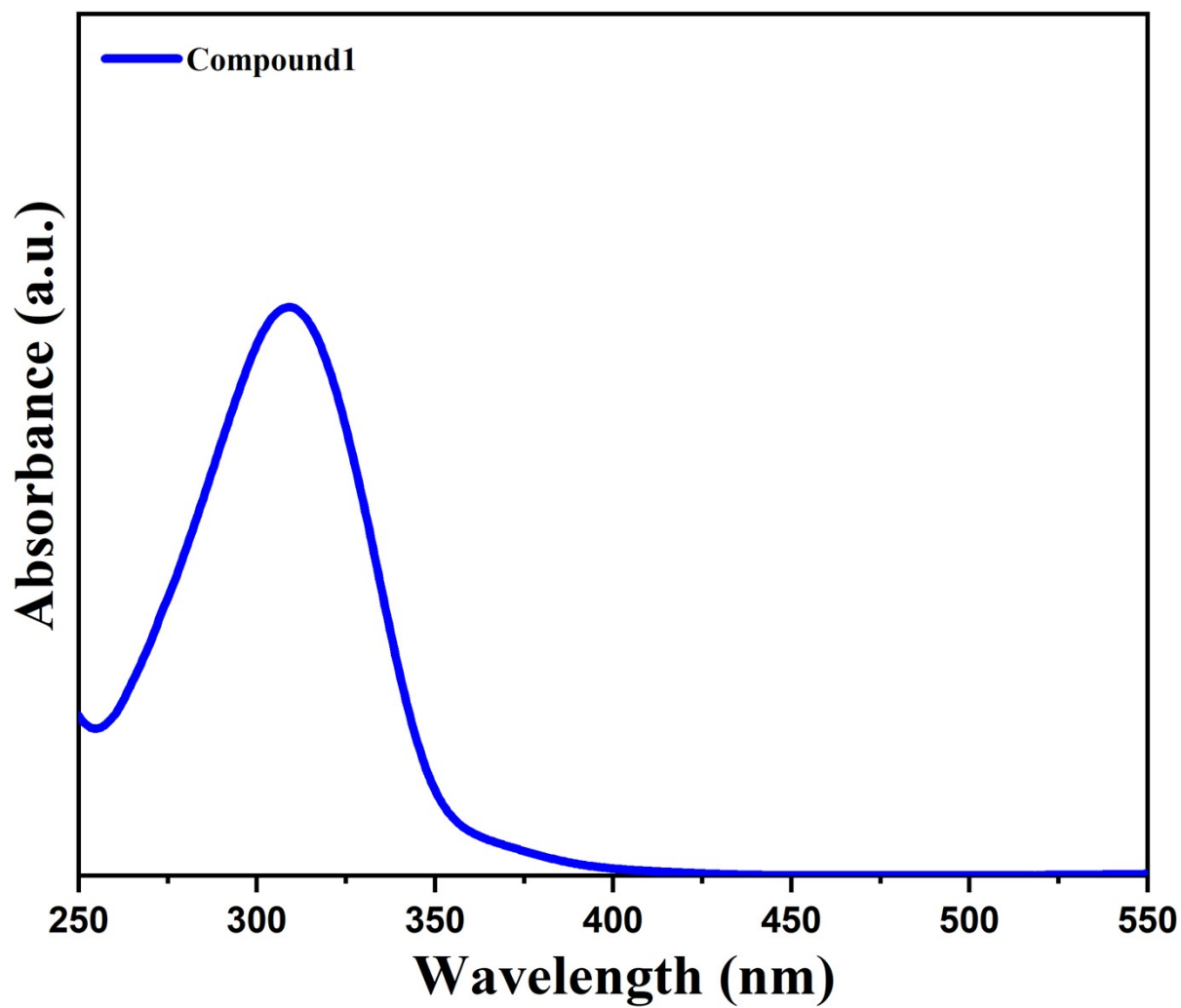


Fig. S15: Absorption spectrum of $[\text{Cd}(\text{PDA})(\text{L})_2]$, 1.

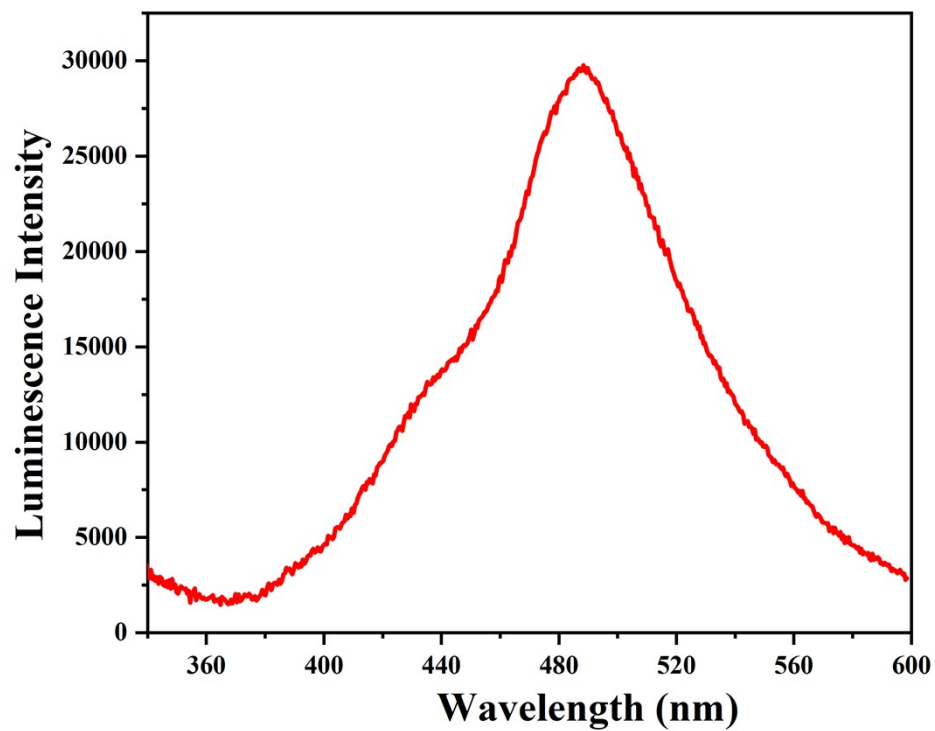


Fig. S16: Emission spectra of **1** in solid state ($\lambda_{\text{ex}} = 300$ nm).

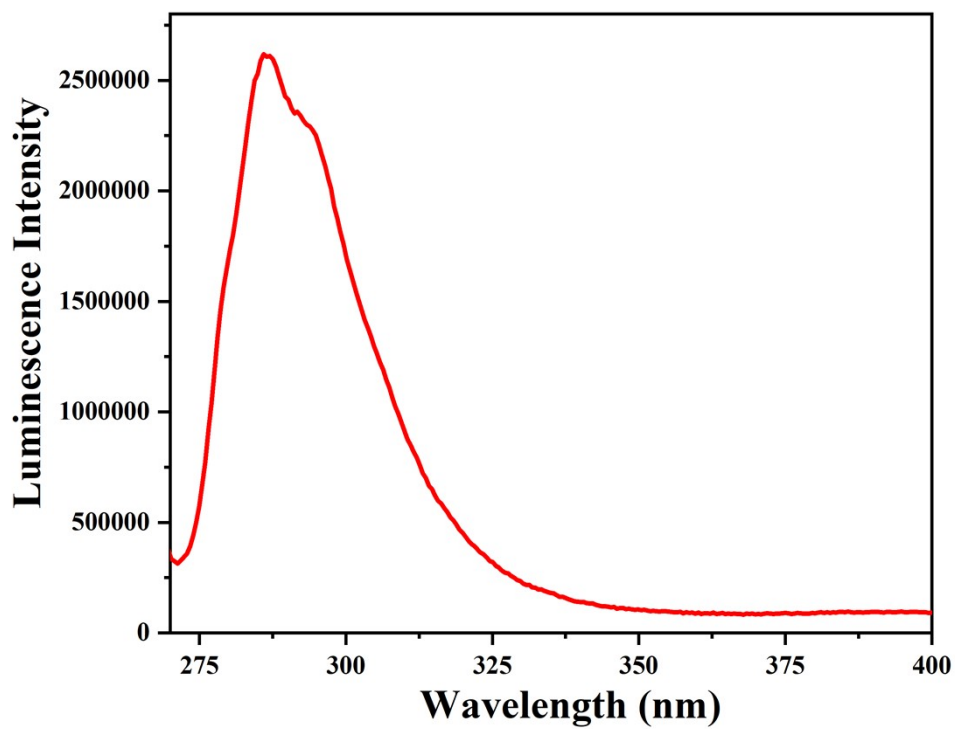


Fig. S17: Emission spectra of 1,4-phenylenediacetic acid in solid state ($\lambda_{\text{ex}} = 263 \text{ nm}$).

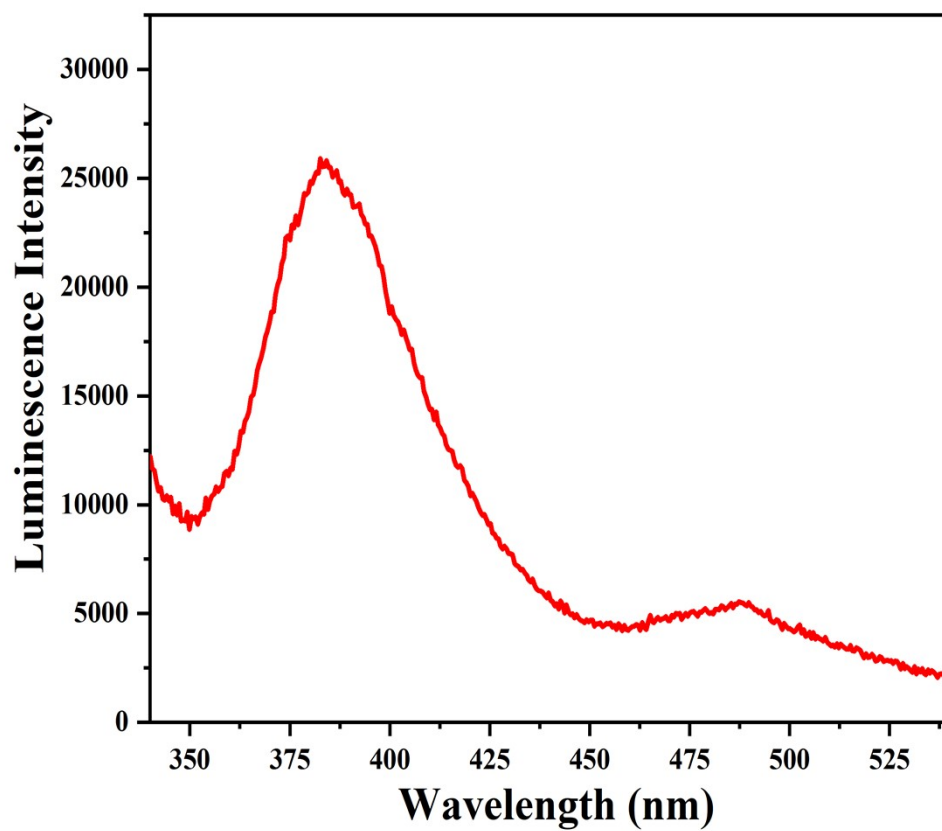


Fig. S18: Emission spectra of 2,4,5-tri-4-pyridyl-1H-imidazole in solid state ($\lambda_{\text{ex}} = 300$ nm).

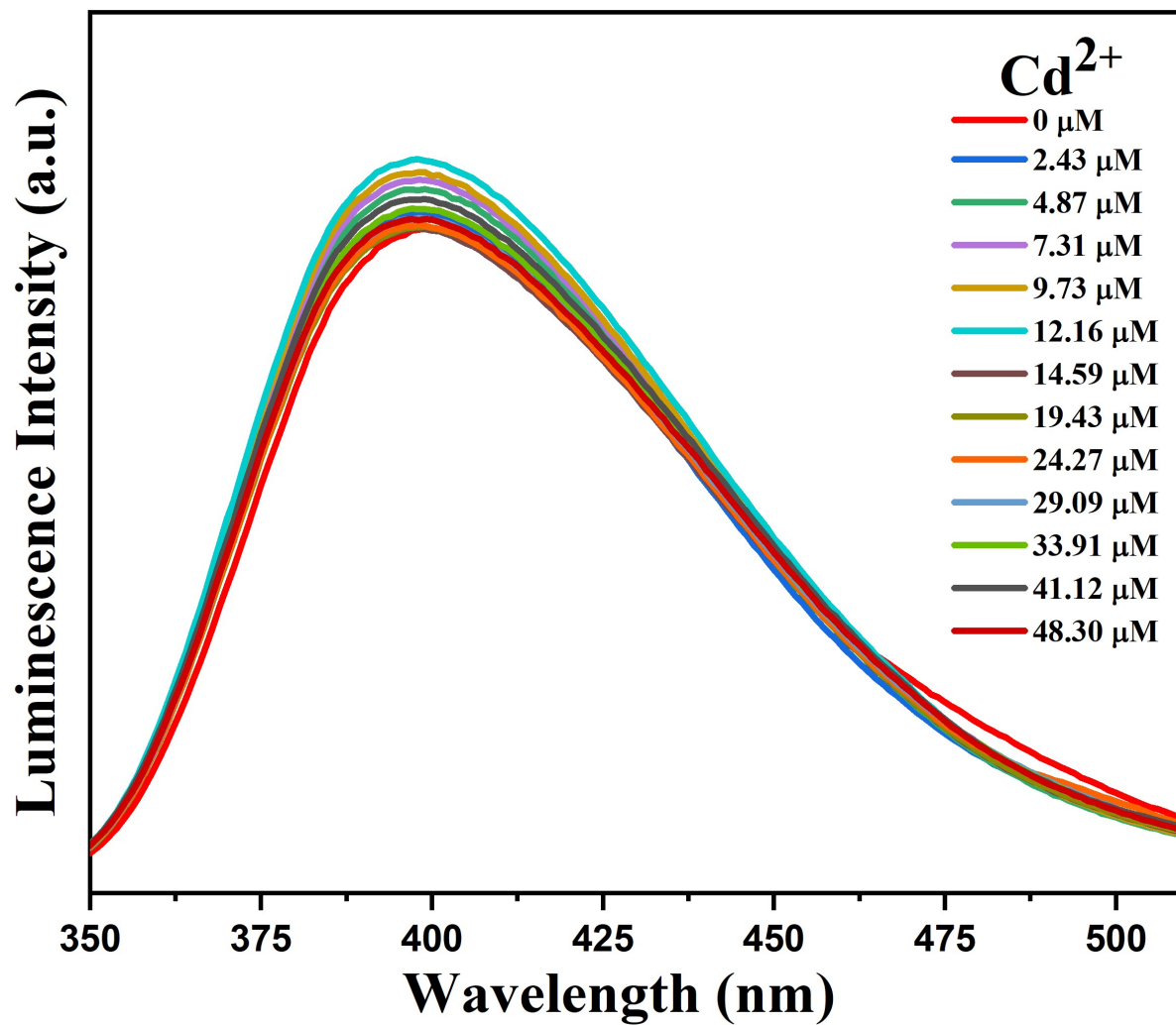


Fig. S19: Emission spectra of **1** dispersed in water upon incremental addition of water solution of Cd²⁺ ions ($\lambda_{\text{ex}} = 300$ nm). Final concentration of Cd²⁺ ions in the medium is indicated in the legend.

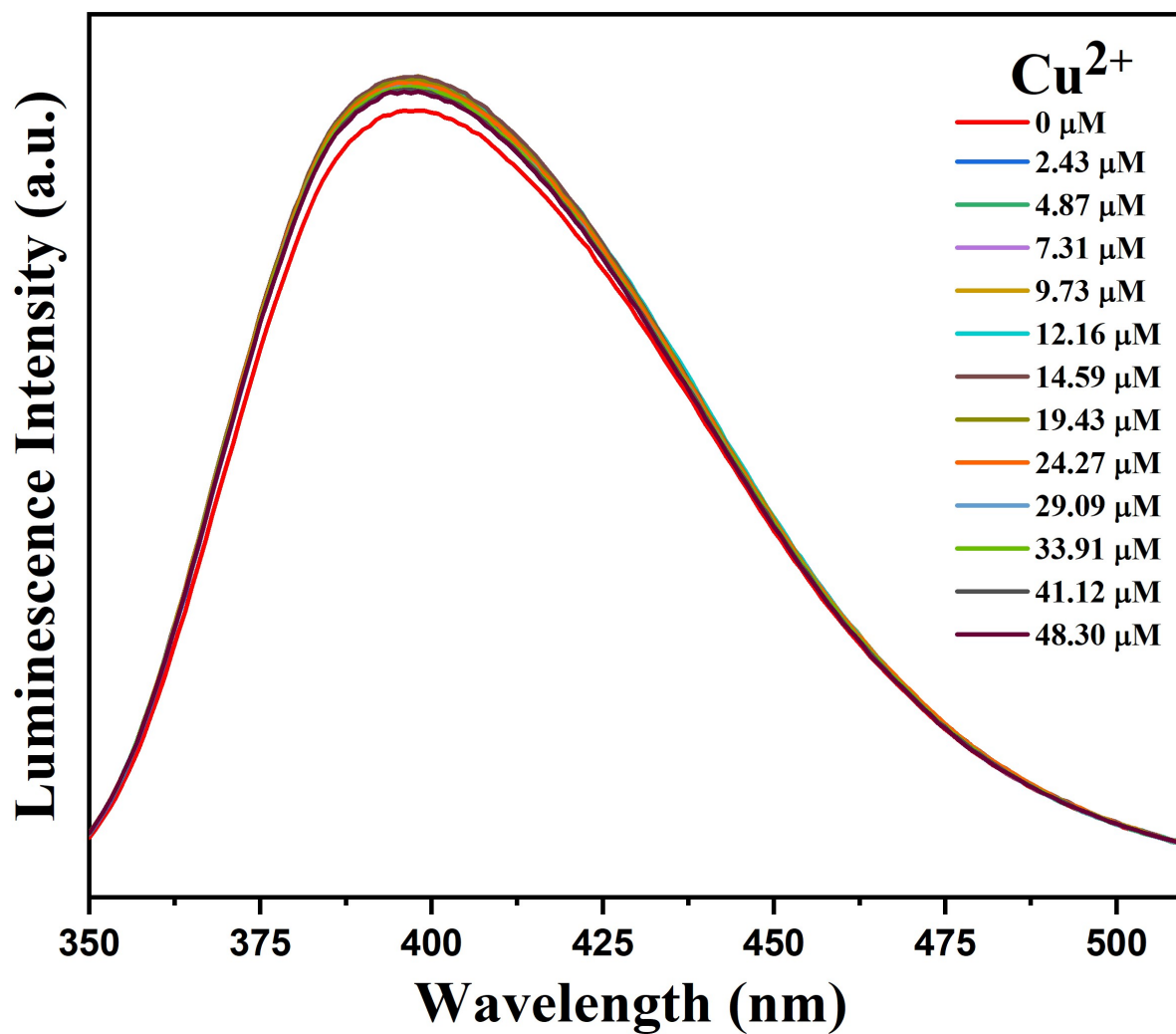


Fig. S20: Emission spectra of **1** dispersed in water upon incremental addition of water solution of Cu²⁺ ions ($\lambda_{\text{ex}} = 300$ nm). Final concentration of Cu²⁺ ions in the medium is indicated in the legend.

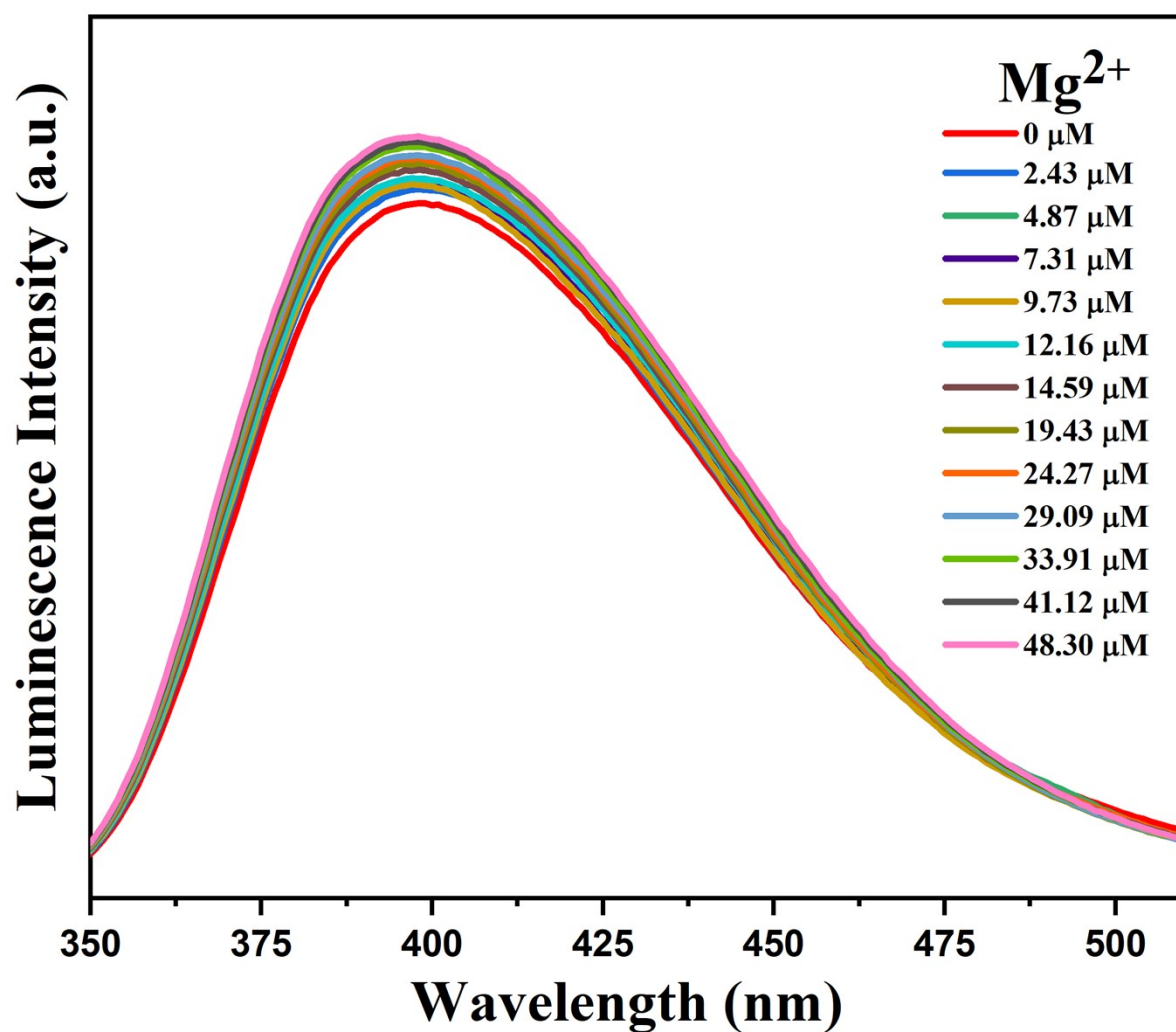


Fig. S21: Emission spectra of **1** dispersed in water upon incremental addition of water solution of Mg^{2+} ions ($\lambda_{\text{ex}} = 300 \text{ nm}$). Final concentration of Mg^{2+} ions in the medium is indicated in the legend.

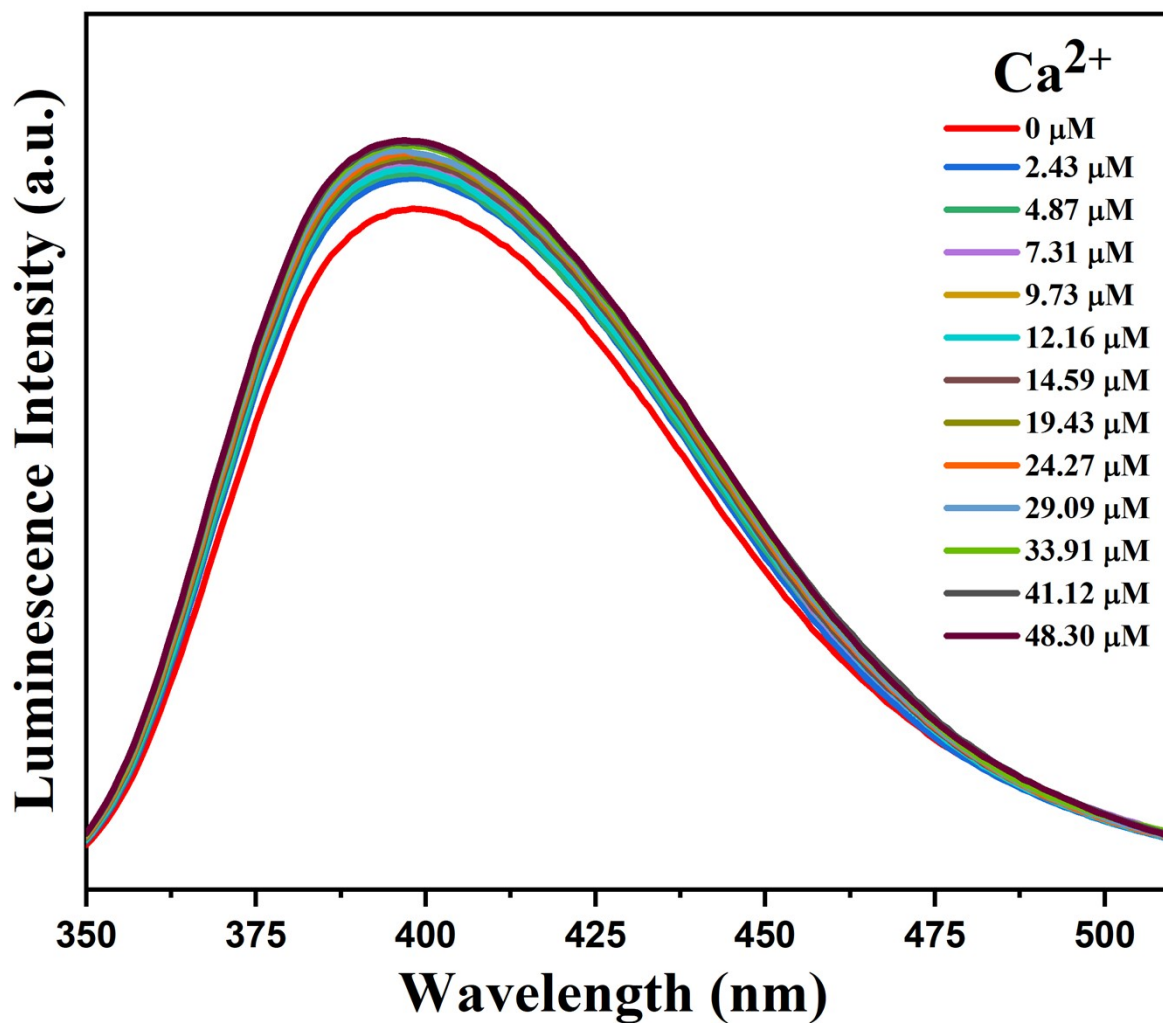


Fig. S22: Emission spectra of **1** dispersed in water upon incremental addition of water solution of Ca²⁺ ions ($\lambda_{\text{ex}} = 300$ nm). Final concentration of Ca²⁺ ions in the medium is indicated in the legend.

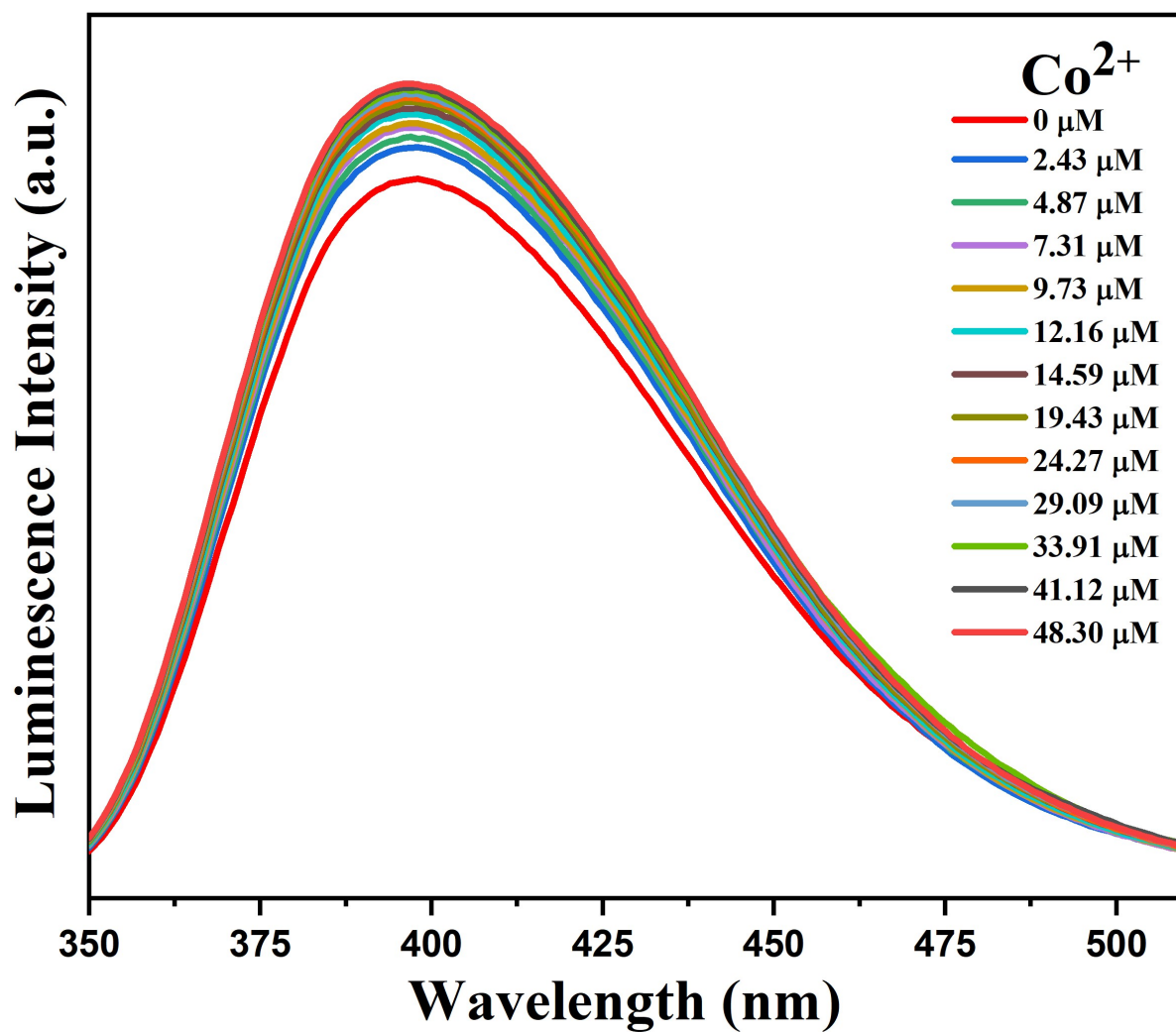


Fig. S23: Emission spectra of 1 dispersed in water upon incremental addition of water solution of Co^{2+} ions ($\lambda_{\text{ex}} = 300 \text{ nm}$). Final concentration of Co^{2+} ions in the medium is indicated in the legend.

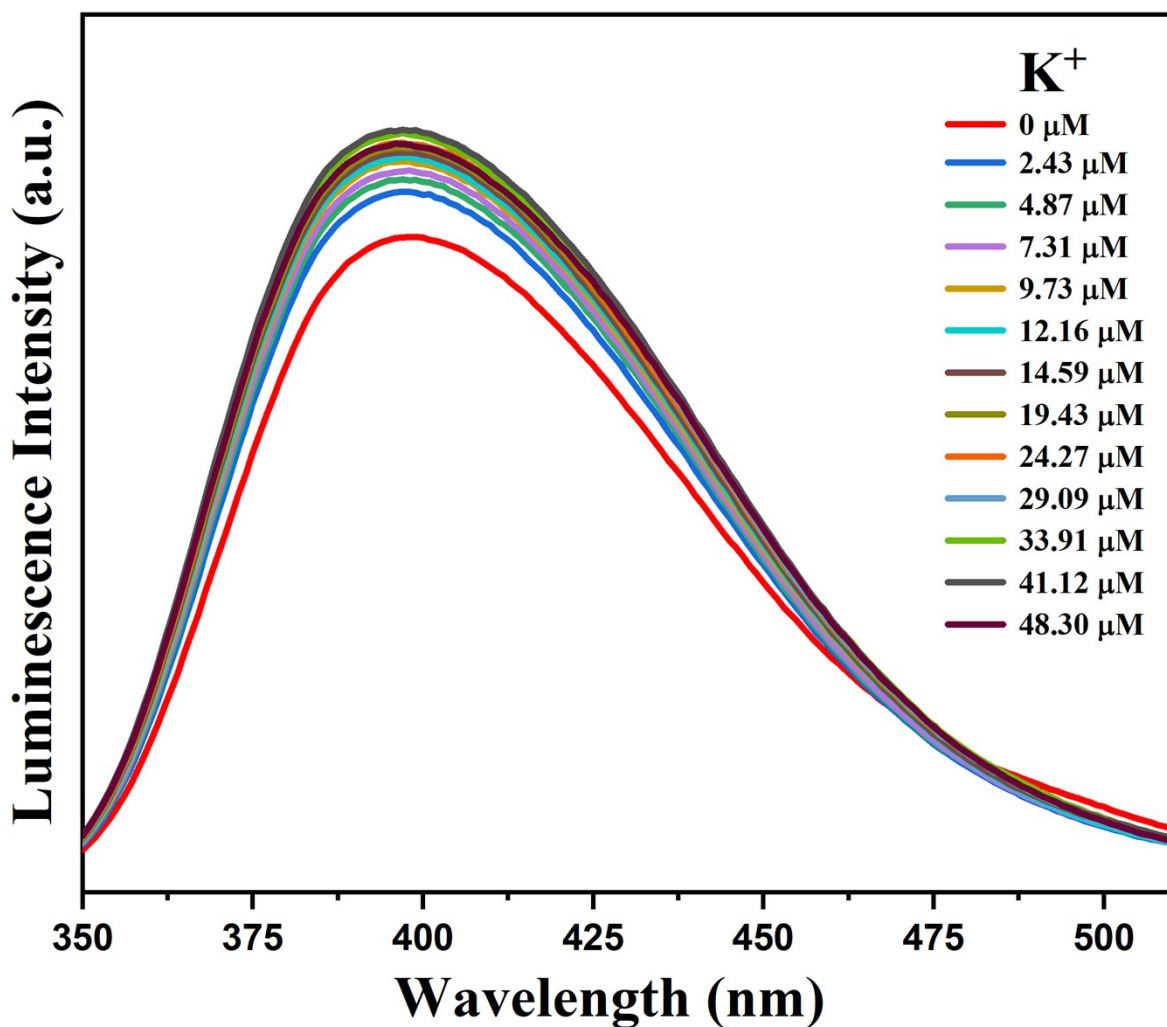


Fig. S24: Emission spectra of **1** dispersed in water upon incremental addition of water solution of K^+ ions ($\lambda_{\text{ex}} = 300 \text{ nm}$). Final concentration of K^+ ions in the medium is indicated in the legend.

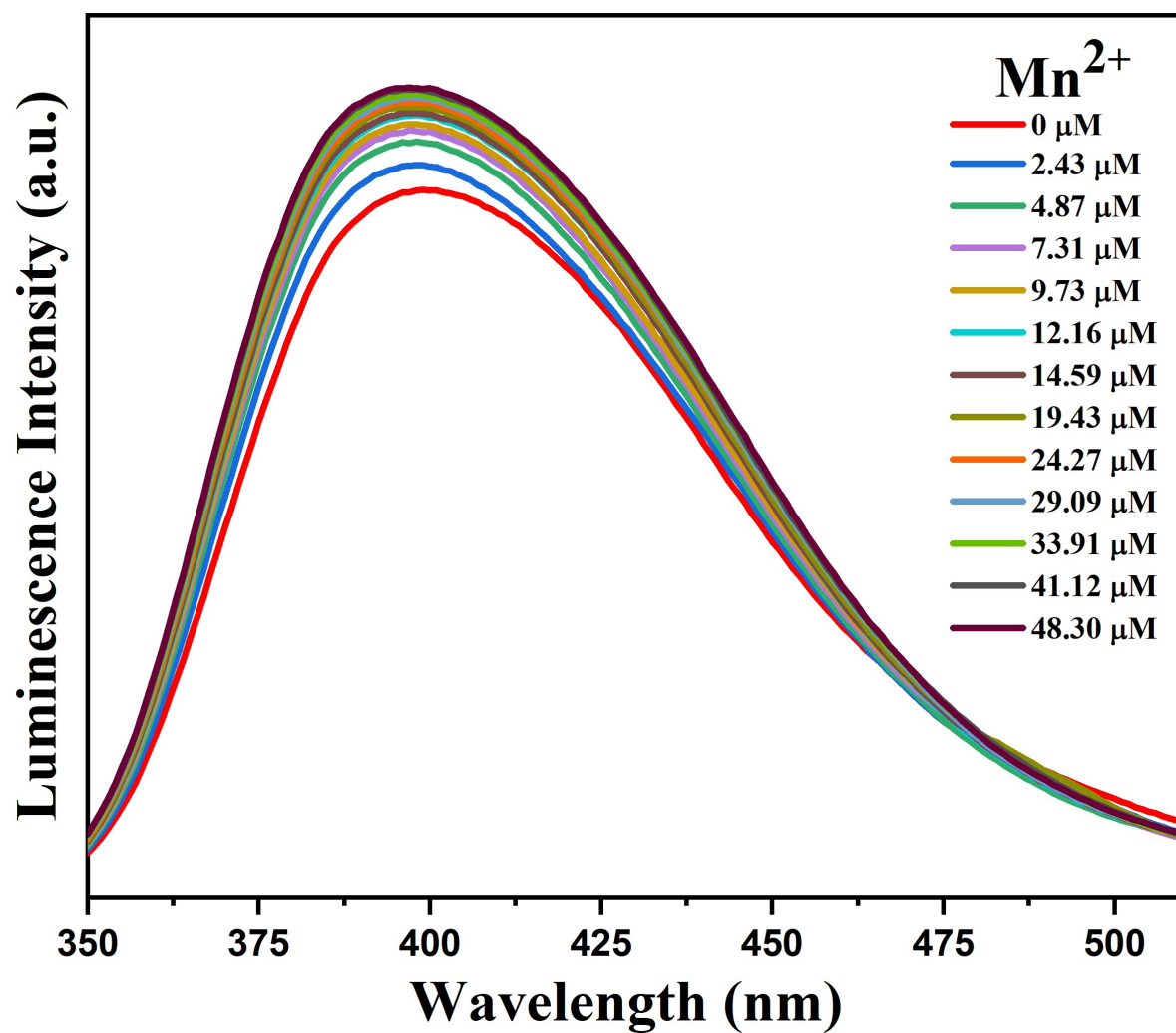


Fig. S25: Emission spectra of 1 dispersed in water upon incremental addition of water solution of Mn²⁺ ions ($\lambda_{\text{ex}} = 300 \text{ nm}$). Final concentration of Mn²⁺ ions in the medium is indicated in the legend.

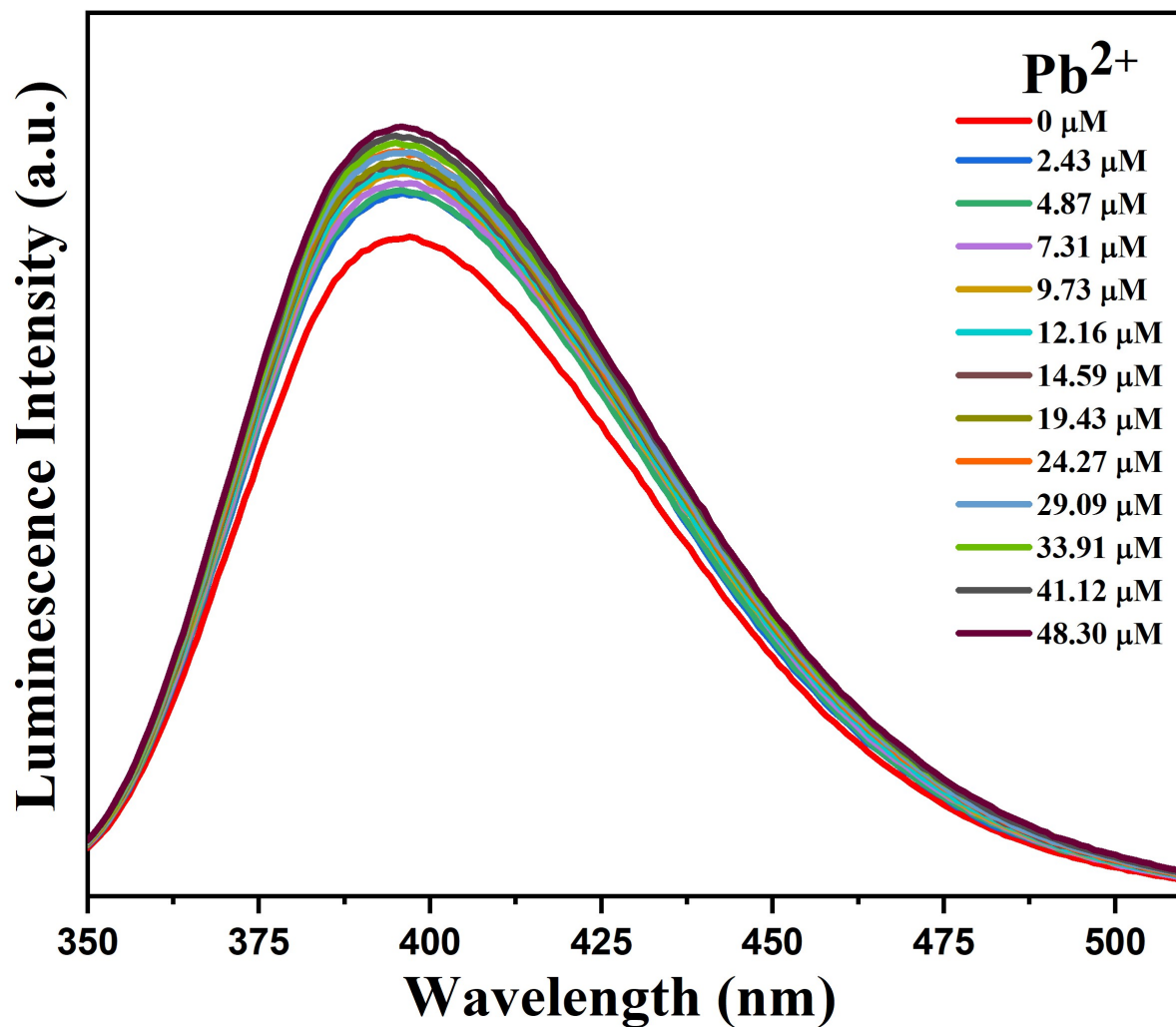


Fig. S26: Emission spectra of **1** dispersed in water upon incremental addition of water solution of Pb²⁺ ions ($\lambda_{\text{ex}} = 300$ nm). Final concentration of Pb²⁺ ions in the medium is indicated in the legend.

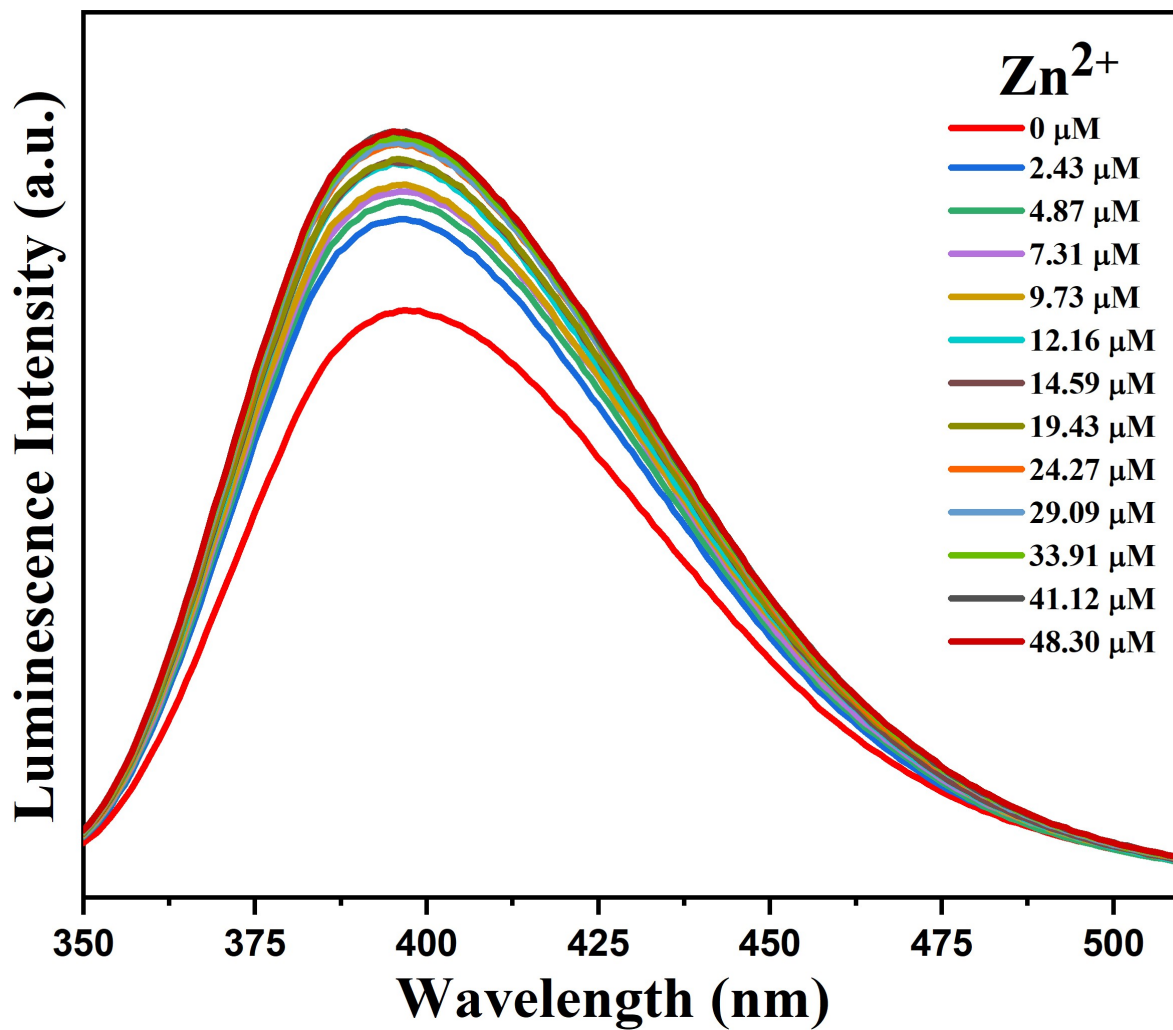


Fig. S27: Emission spectra of **1** dispersed in water upon incremental addition of water solution of Zn²⁺ ions ($\lambda_{\text{ex}} = 300$ nm). Final concentration of Zn²⁺ ions in the medium is indicated in the legend.

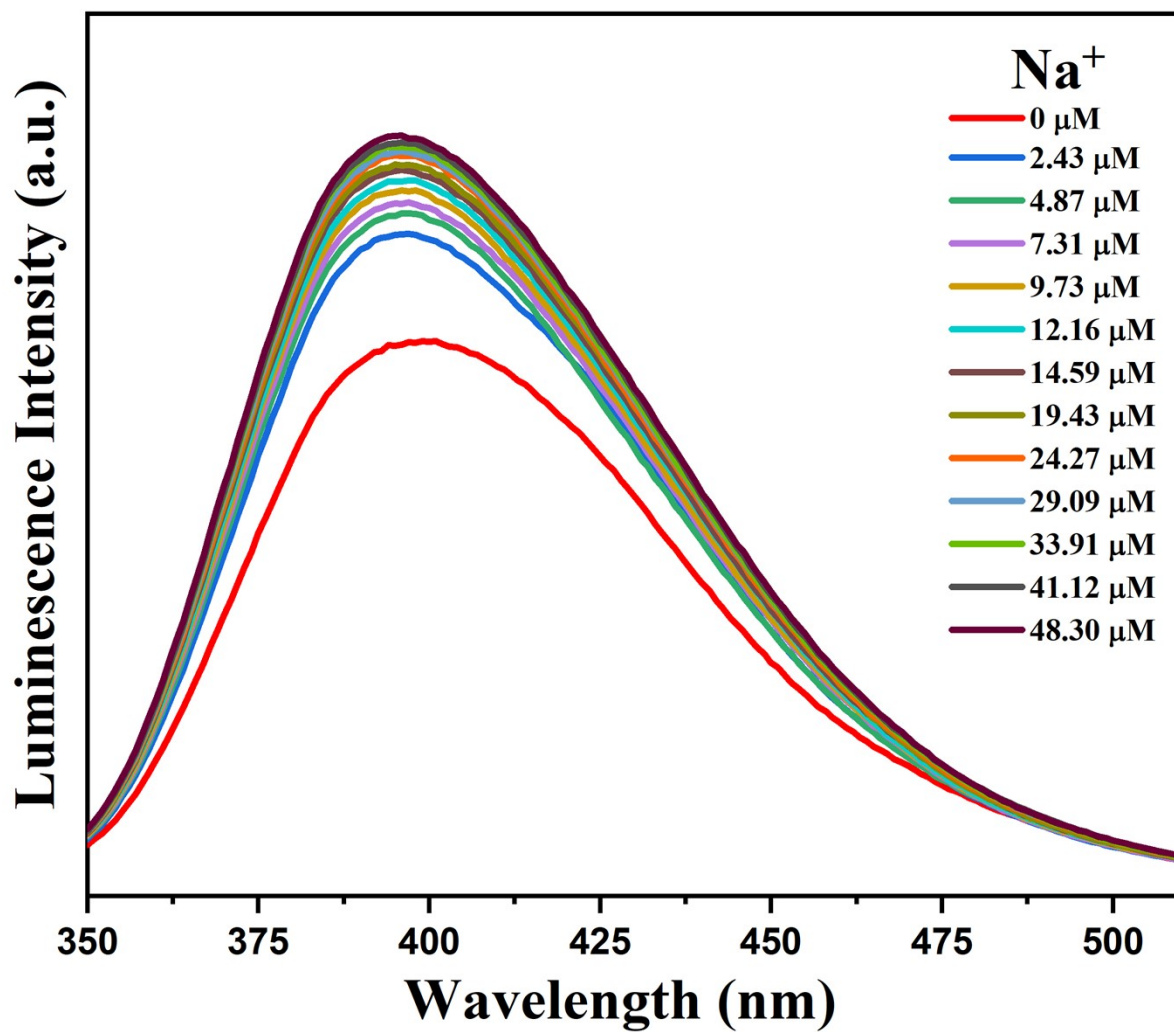


Fig. S28: Emission spectra of **1** dispersed in water upon incremental addition of water solution of Na⁺ ions ($\lambda_{\text{ex}} = 300$ nm). Final concentration of Na⁺ ions in the medium is indicated in the legend.

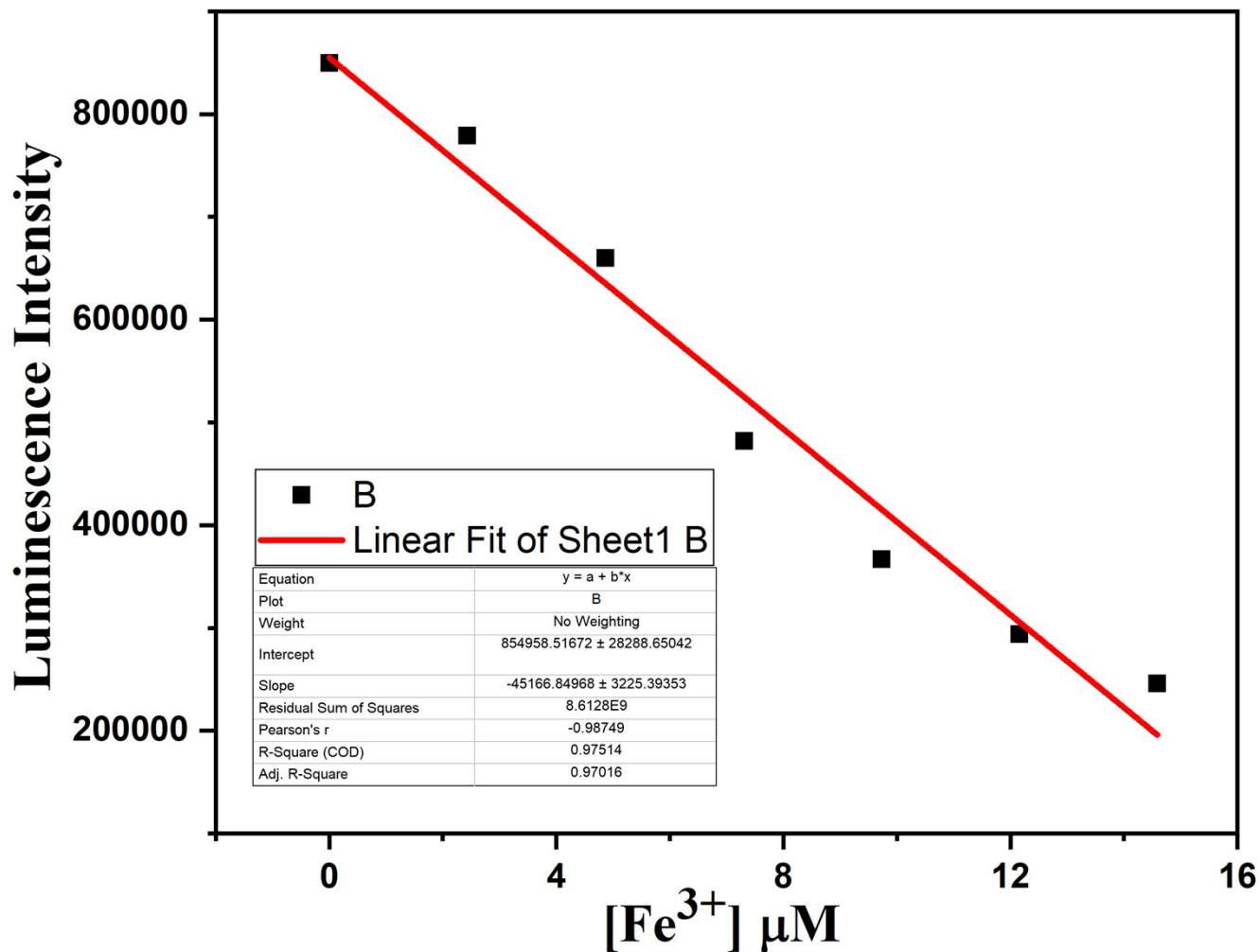


Fig. S29: The plot of the changes of luminescence intensity of compound **1** ($\lambda_{em} = 398$ nm) vs concentration of Fe^{3+} solution (upto 14.59 μM) indicating the detection limit, which calculated using the equation, $LOD = 3\sigma/m$, where σ = standard deviation of blank determination and m = slope of the linear curve.

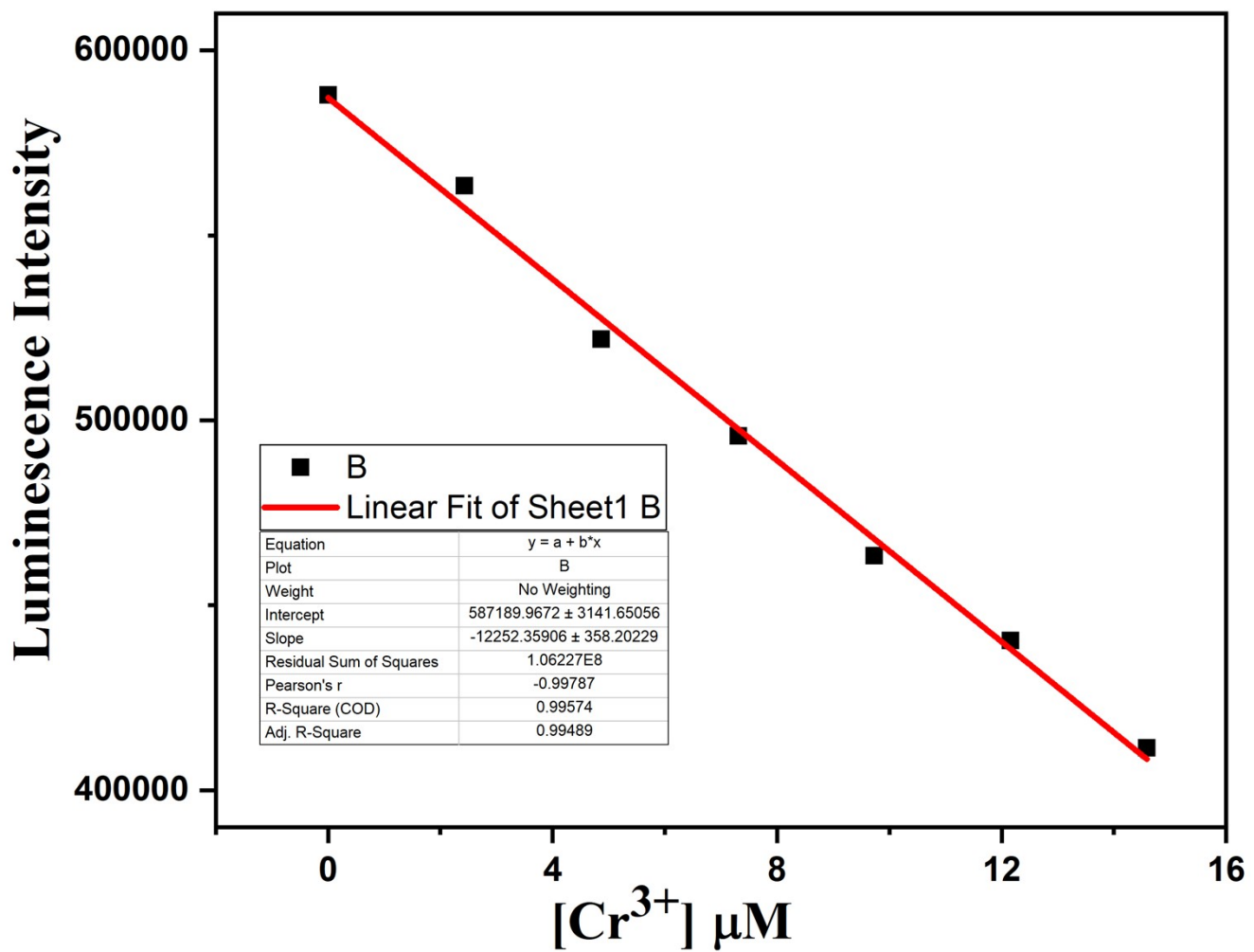


Fig. S30: The plot of the changes of luminescence intensity of compound **1** ($\lambda_{em} = 398$ nm) vs concentration of Cr^{3+} solution (upto 14.59 μM) indicating the detection limit, which calculated using the equation, $LOD = 3\sigma/m$, where σ = standard deviation of blank determination and m = slope of the linear curve.

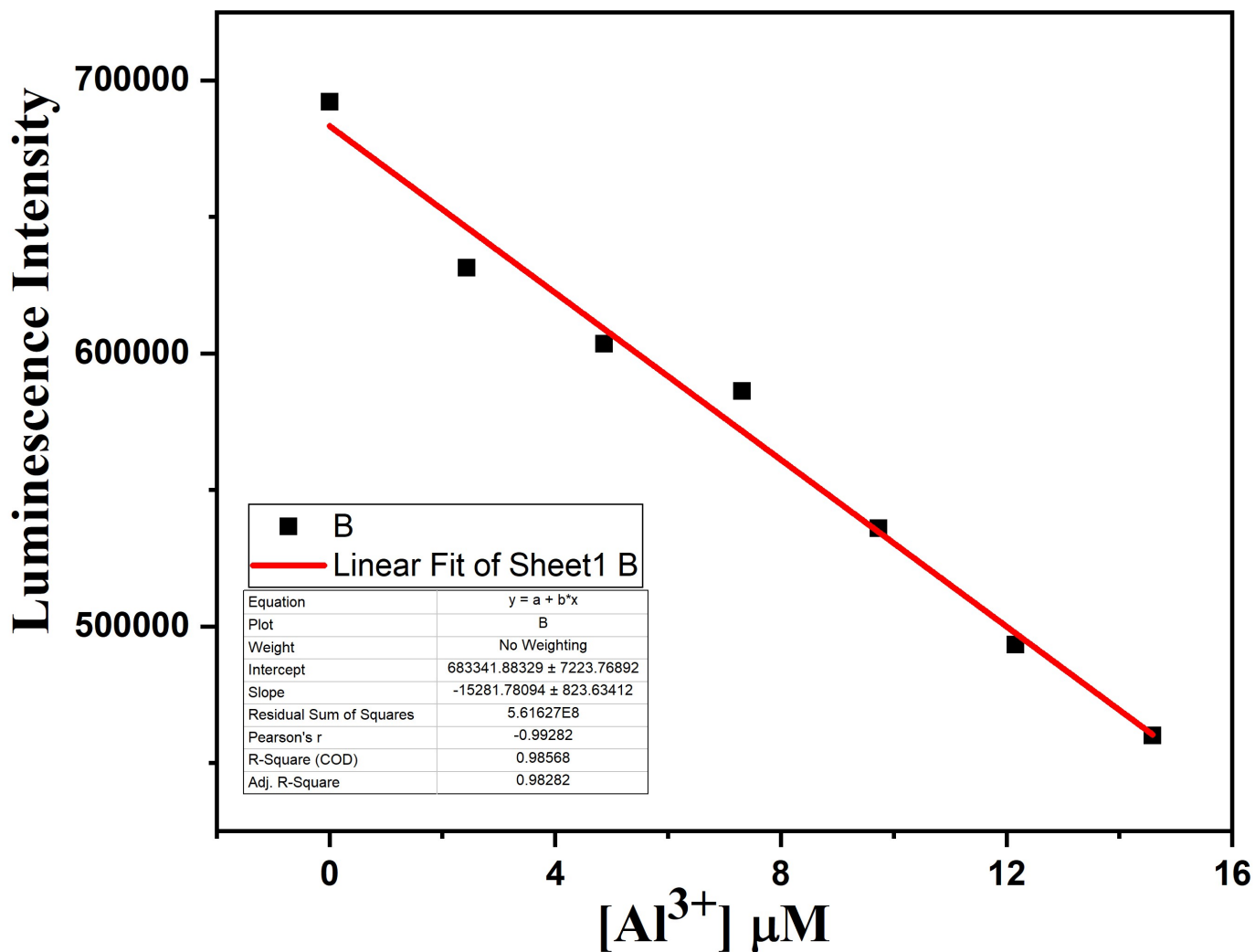


Fig. S31: The plot of the changes of luminescence intensity of compound **1** ($\lambda_{em} = 398$ nm) vs concentration of Al^{3+} solution (upto $14.59 \mu M$) indicating the detection limit, which calculated using the equation, $LOD = 3\sigma/m$, where σ = standard deviation of blank determination and m = slope of the linear curve.

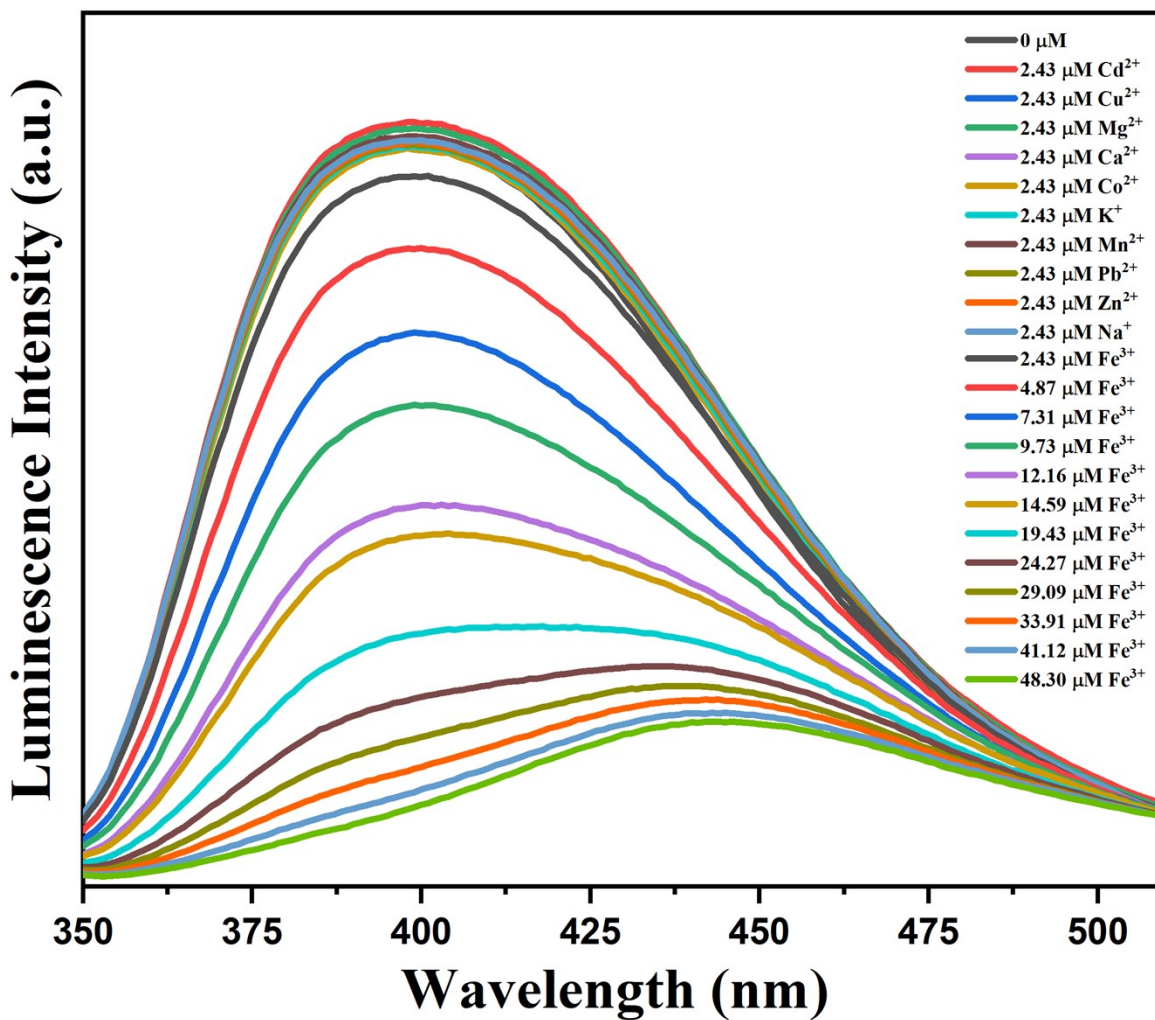


Fig. S32: Emission spectra of **1** dispersed in water upon incremental addition of Fe³⁺ solution in the presence of 2.43 μM concentration of various metal ions ($\lambda_{\text{ex}} = 300$ nm).

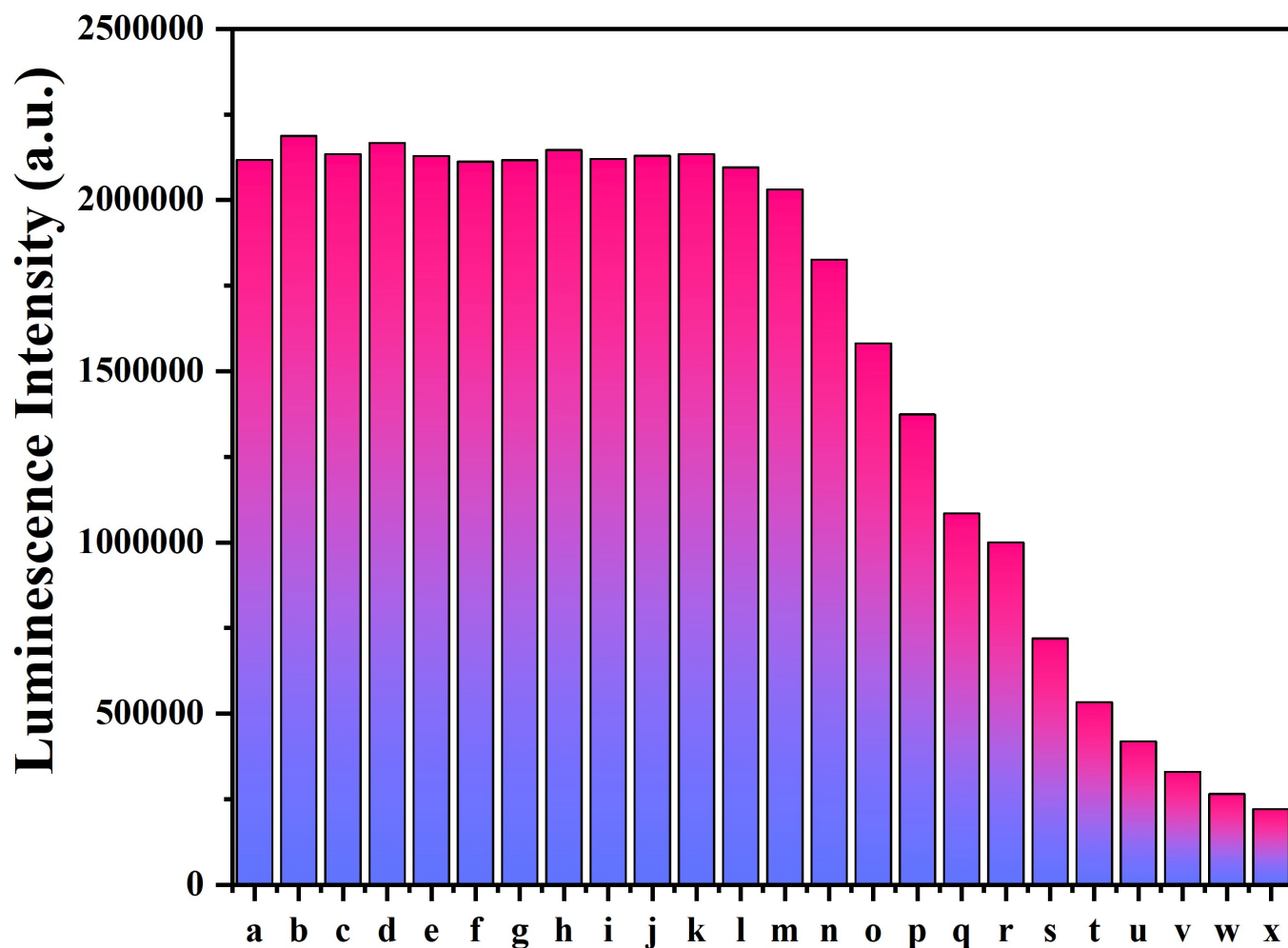


Fig. S33: Bar diagram presenting the luminescence intensity (observed at 398 nm) after the consecutive addition of the analytes. The composition and concentration of the system were as follows: (a) **1** in aqueous dispersion, (b) a + 2.43 μM Cd^{2+} , (c) b + 2.43 μM Cu^{2+} , (d) c + 2.43 μM Mg^{2+} , (e) d + 2.43 μM Ca^{2+} , (f) e + 2.43 μM Co^{2+} , (g) f + 2.43 μM K^{+} , (h) g + 2.43 μM Mn^{2+} , (i) h + 2.43 μM Pb^{2+} , (j) i + 2.43 μM Zn^{2+} , (k) j + 2.43 μM Na^{+} , (l) k + 2.43 μM Fe^{3+} , (m) l + 2.43 μM Fe^{3+} , (n) m + 2.43 μM Fe^{3+} , (o) n + 2.43 μM Fe^{3+} , (p) o + 2.43 μM Fe^{3+} , (q) p + 2.43 μM Fe^{3+} , (r) q + 4.87 μM Fe^{3+} , (s) r + 4.87 μM Fe^{3+} , (t) s + 4.87 μM Fe^{3+} , (u) q + 4.87 μM Fe^{3+} , (v) r + 4.87 μM Fe^{3+} , (w) s + 7.31 μM Fe^{3+} , and (x) s + 7.31 μM Fe^{3+} .

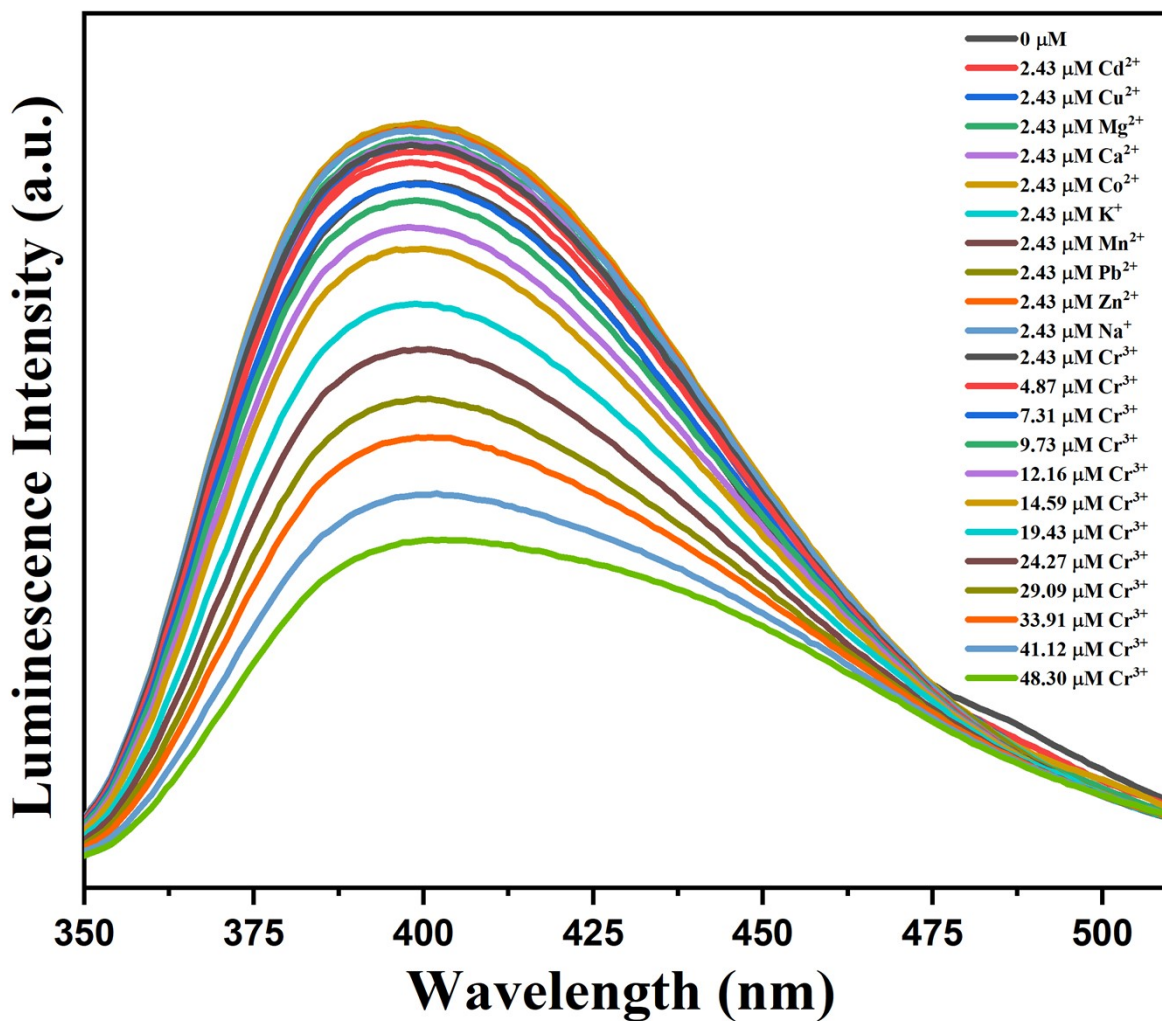


Fig. S34: Emission spectra of 1 dispersed in water upon incremental addition of Cr³⁺ solution in the presence of 2.43 μM concentration of various metal ions ($\lambda_{\text{ex}} = 300 \text{ nm}$).

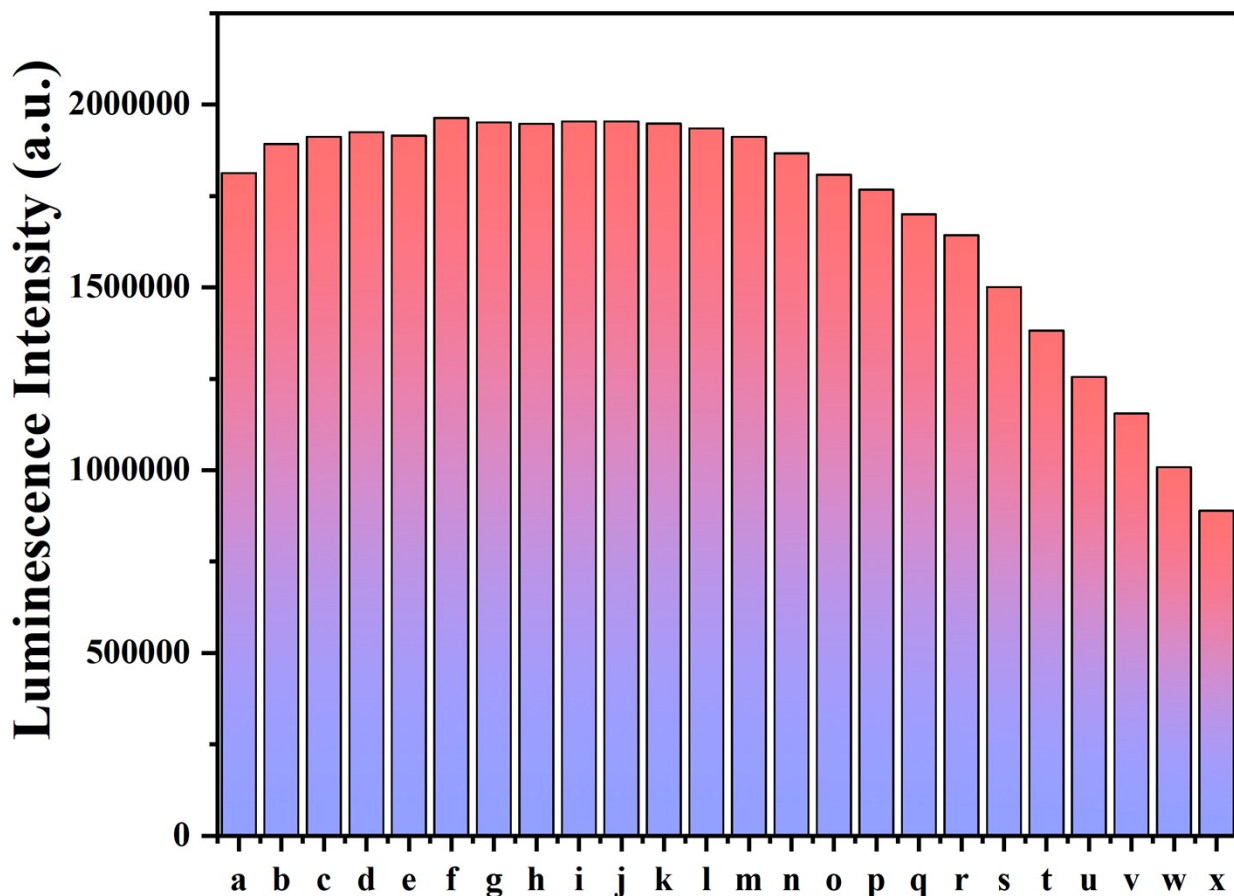


Fig. S35: Bar diagram presenting the luminescence intensity (observed at 398 nm) after the consecutive addition of the analytes. The composition and concentration of the system were as follows: (a) **1** in aqueous dispersion, (b) a + 2.43 μM Cd^{2+} , (c) b + 2.43 μM Cu^{2+} , (d) c + 2.43 μM Mg^{2+} , (e) d + 2.43 μM Ca^{2+} , (f) e + 2.43 μM Co^{2+} , (g) f + 2.43 μM K^{+} , (h) g + 2.43 μM Mn^{2+} , (i) h + 2.43 μM Pb^{2+} , (j) i + 2.43 μM Zn^{2+} , (k) j + 2.43 μM Na^{+} , (l) k + 2.43 μM Cr^{3+} , (m) l + 2.43 μM Cr^{3+} , (n) m + 2.43 μM Cr^{3+} , (o) n + 2.43 μM Cr^{3+} , (p) o + 2.43 μM Cr^{3+} , (q) p + 2.43 μM Cr^{3+} , (r) q + 4.87 μM Cr^{3+} , (s) r + 4.87 μM Cr^{3+} , (t) s + 4.87 μM Cr^{3+} , (u) q + 4.87 μM Cr^{3+} , (v) r + 4.87 μM Cr^{3+} , (w) s + 7.31 μM Cr^{3+} , and (x) s + 7.31 μM Cr^{3+} .

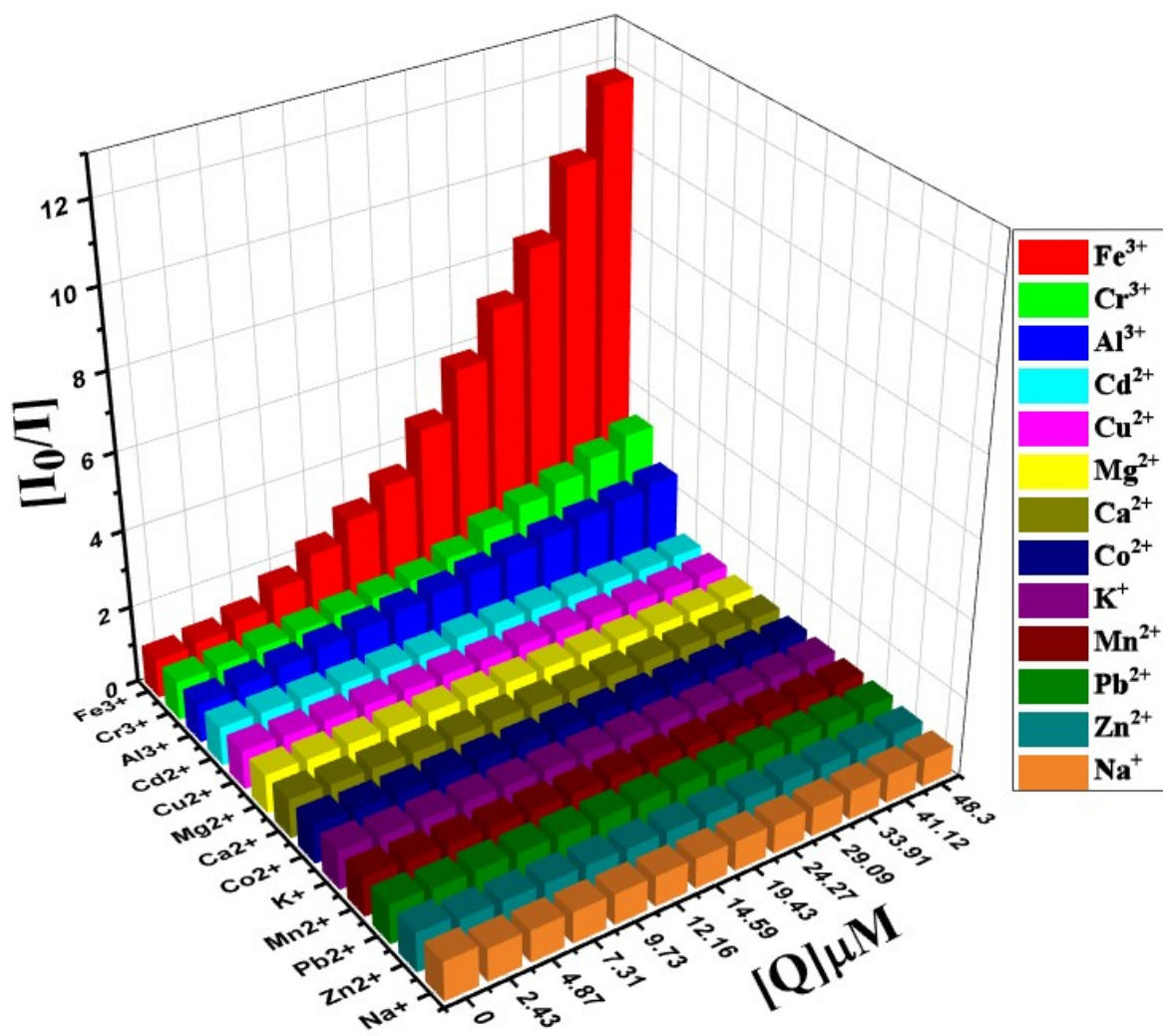


Fig. 36: Stern-Volmer plots of various metal ions in higher concentration range (upto 48.30 μM) for compound 1.

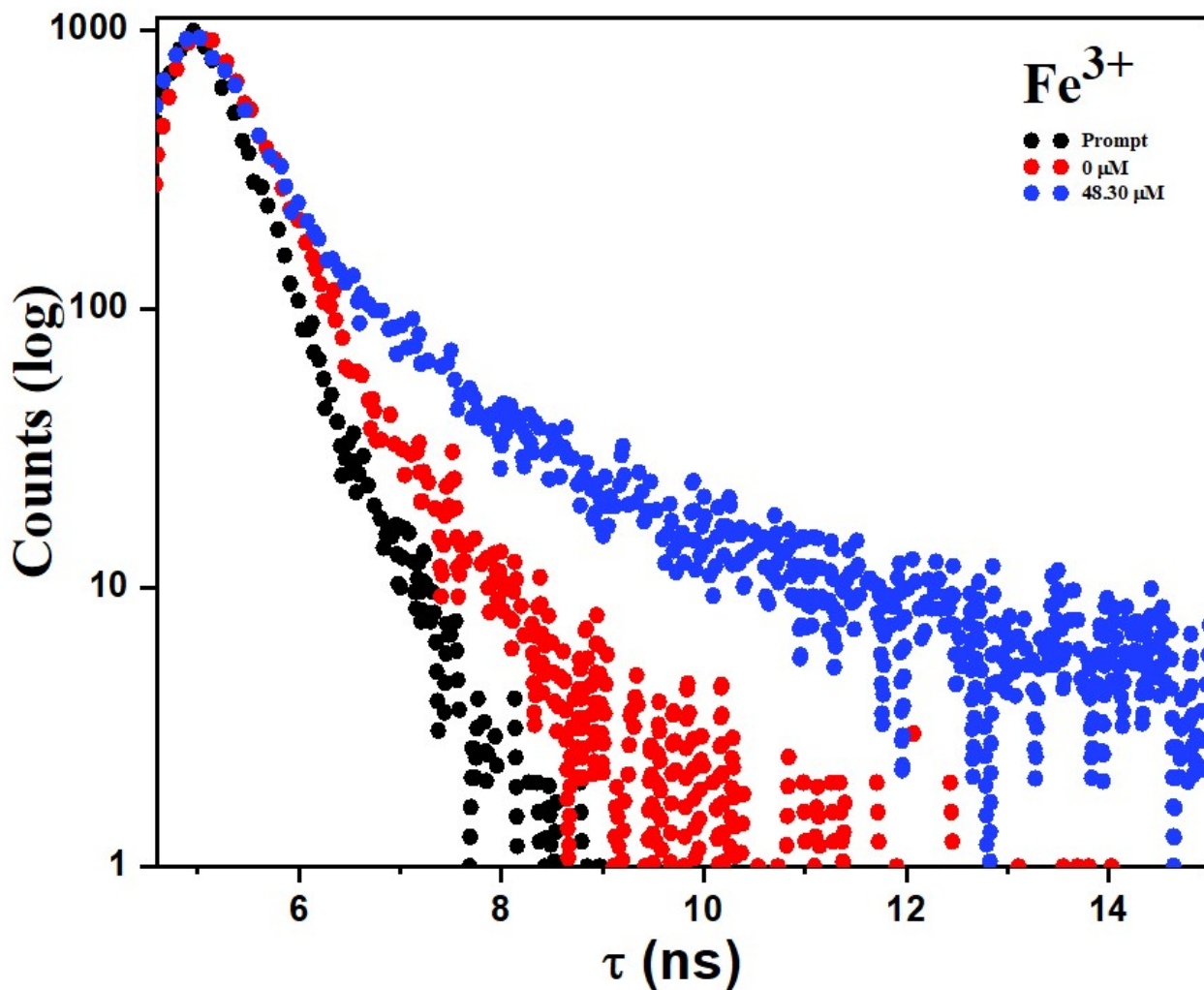


Fig. S37: Luminescence lifetime decay profile of compound **1** before and after the addition of the Fe^{3+} ions. The final concentration of Fe^{3+} ions in the medium is indicated in the legend. The instrument response function (prompt) is also shown. Here, $\lambda_{\text{ex}} = 300$ nm and $\lambda_{\text{em}} = 398$ nm were set during the experiment.

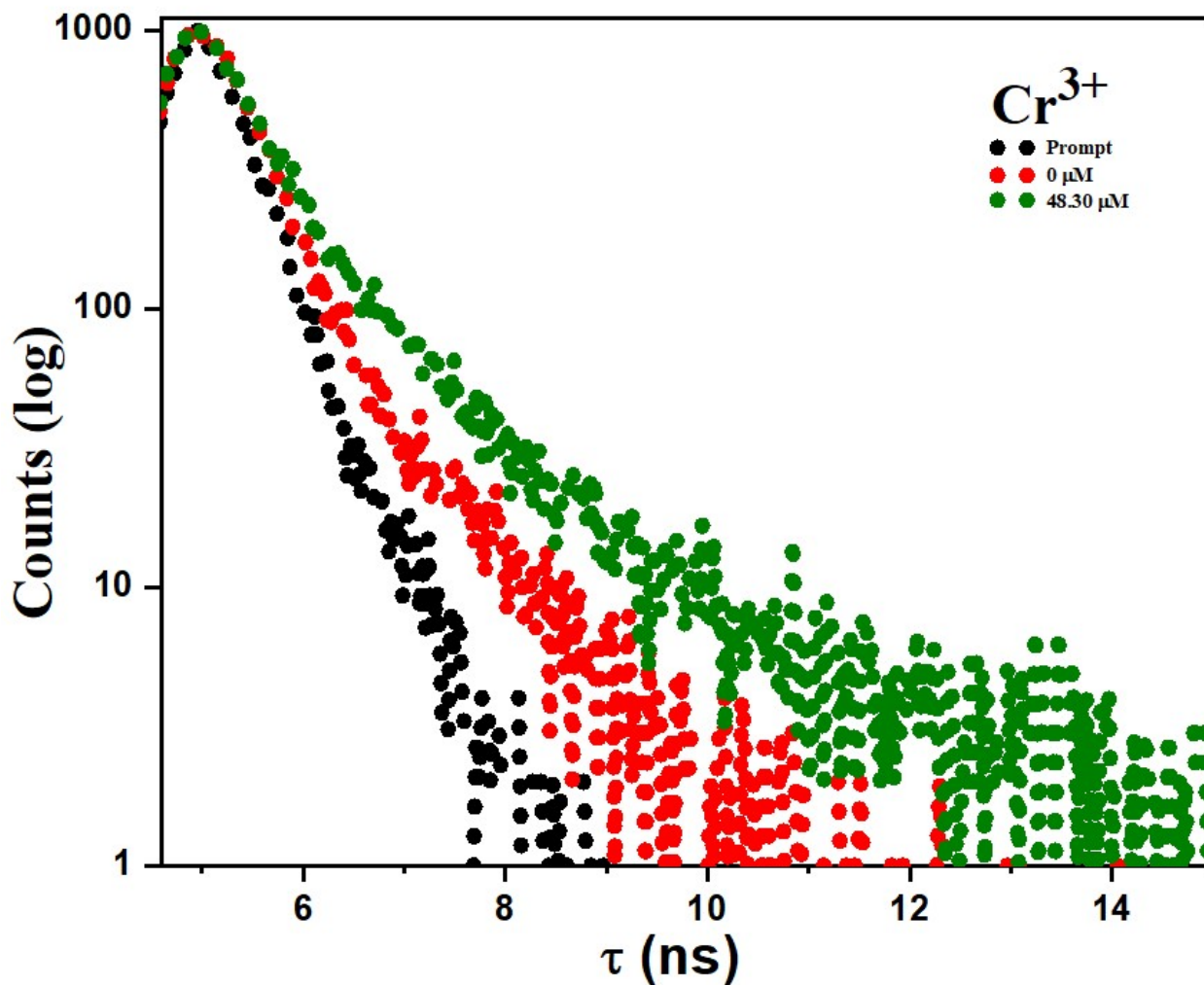


Fig. S38: Luminescence lifetime decay profile of compound **1** before and after the addition of the Cr^{3+} ions. The final concentration of Cr^{3+} ions in the medium is indicated in the legend. The instrument response function (prompt) is also shown. Here, $\lambda_{\text{ex}} = 300 \text{ nm}$ and $\lambda_{\text{em}} = 398 \text{ nm}$ were set during the experiment.

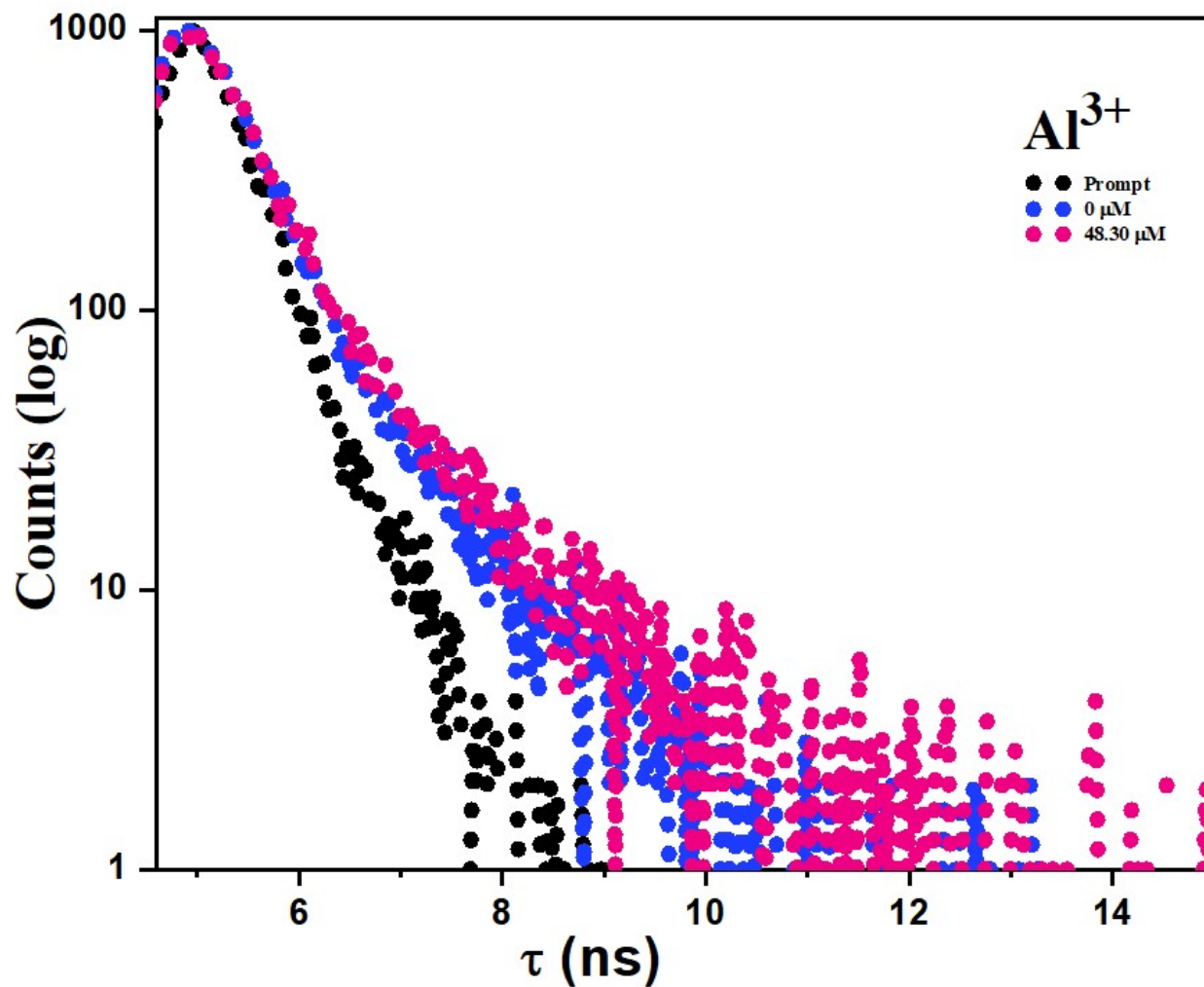


Fig. S39: Luminescence lifetime decay profile of compound **1** before and after the addition of the Al^{3+} ions. The final concentration of Al^{3+} ions in the medium is indicated in the legend. The instrument response function (prompt) is also shown. Here, $\lambda_{\text{ex}} = 300$ nm and $\lambda_{\text{em}} = 398$ nm were set during the experiment.

Table S5: Details about the time-resolved luminescence decays of compound **1** ($\lambda_{\text{ex}} = 300$ nm and $\lambda_{\text{em}} = 398$ nm) in presence of Fe^{3+} , Cr^{3+} , Al^{3+} solution.

Metal ions	Concentration (μM)	Lifetime (ns)			
		T_1	T_2	$T_{\text{av}} = (T_1+T_2)/2$	$\tau(\text{ns})$
Fe^{3+}	0	0.2030	0	0.101	0.203
	48.30	0.1479	1.2854	0.716	0.344
Cr^{3+}	0	0.2321	0	0.116	0.232
	48.30	0.1590	1.3480	0.753	0.490
Al^{3+}	0	0.2415	0	0.120	0.241
	48.30	0.1322	1.0551	0.593	0.301

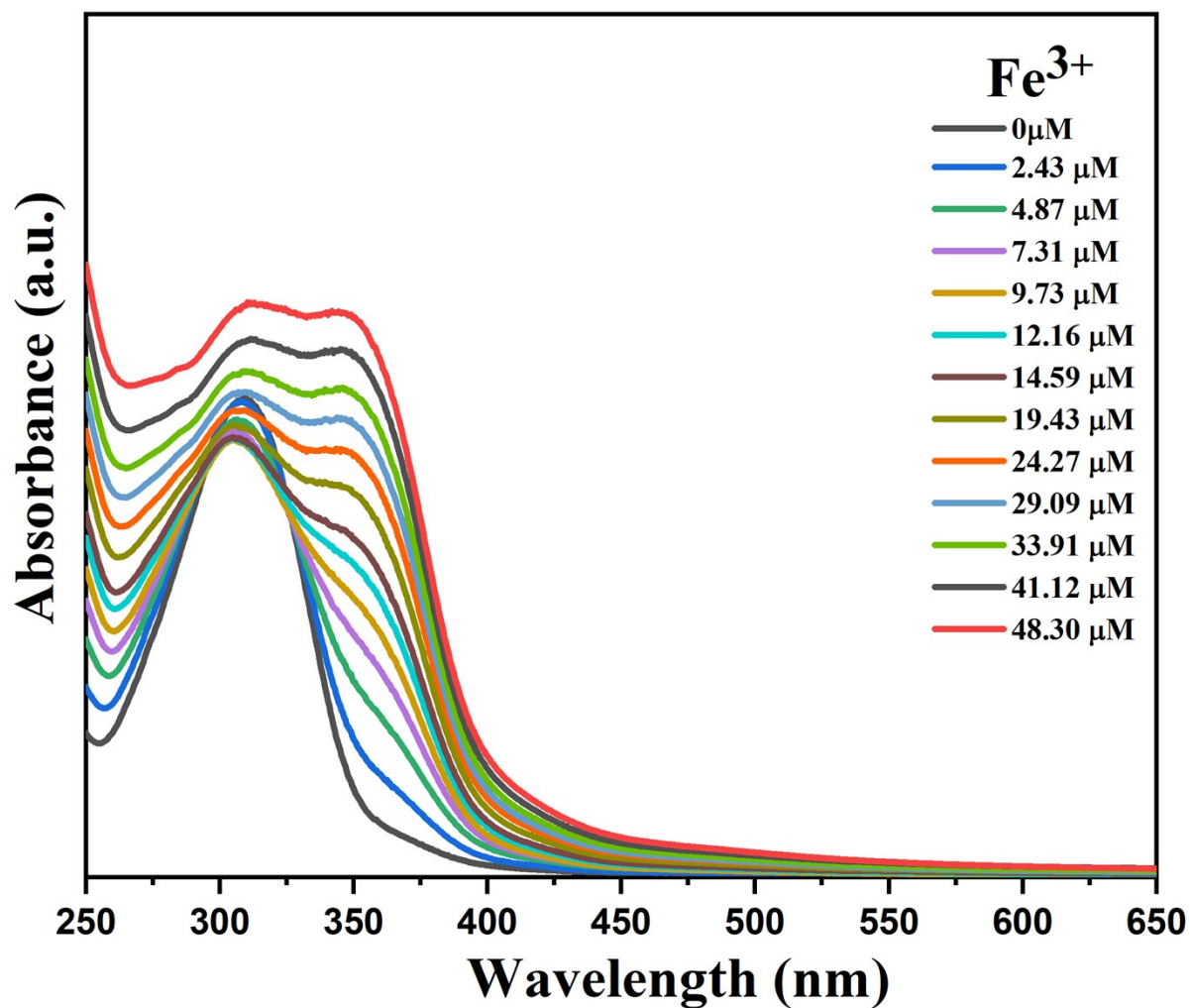


Fig. S40: Absorption spectra of **1** dispersed in water upon incremental addition of water solution of Fe³⁺ ions. Final concentration of Fe³⁺ ions in the medium is indicated in the legend.

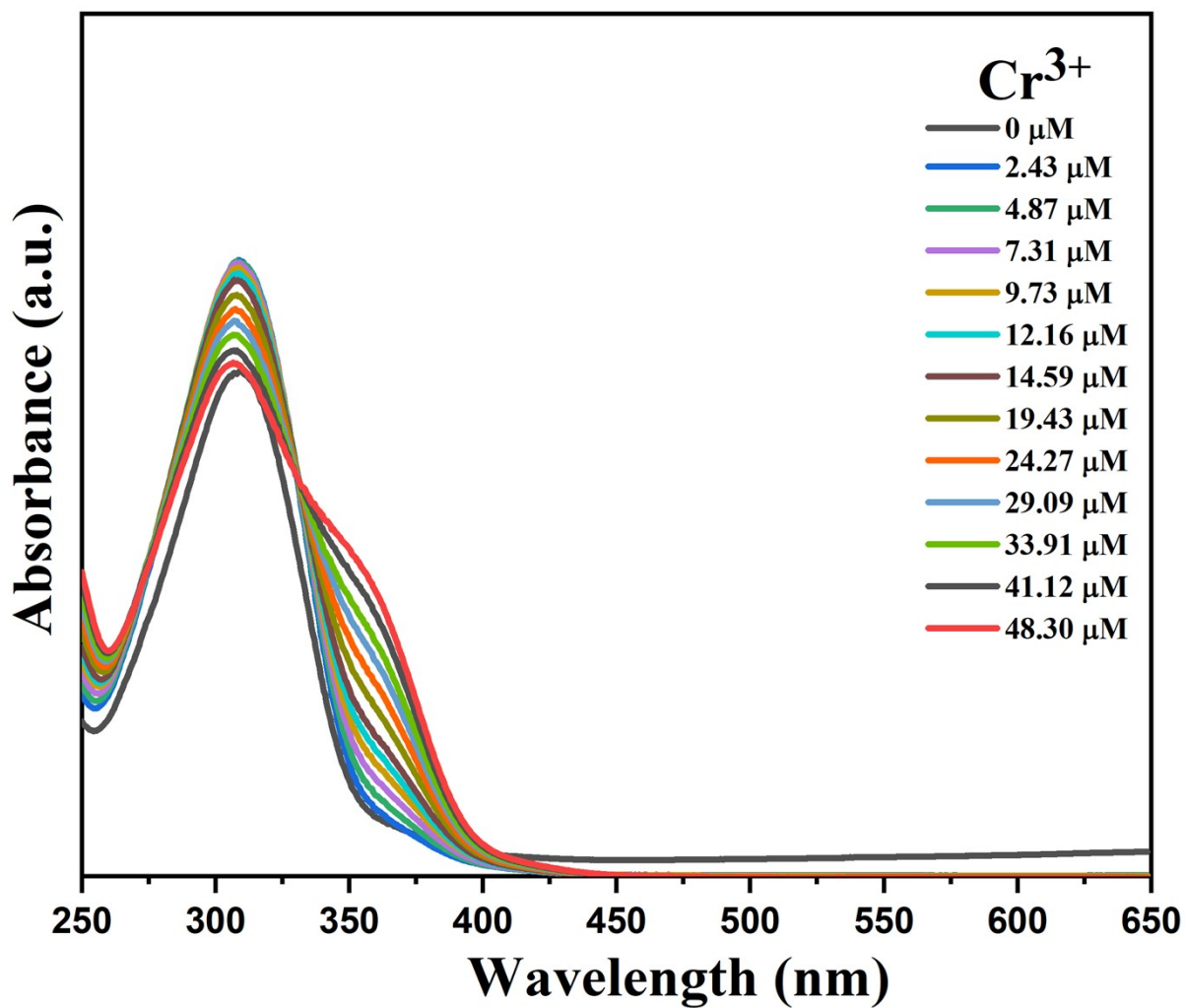


Fig. S41: Absorption spectra of **1** dispersed in water upon incremental addition of water solution of Cr³⁺ ions. Final concentration of Cr³⁺ ions in the medium is indicated in the legend.

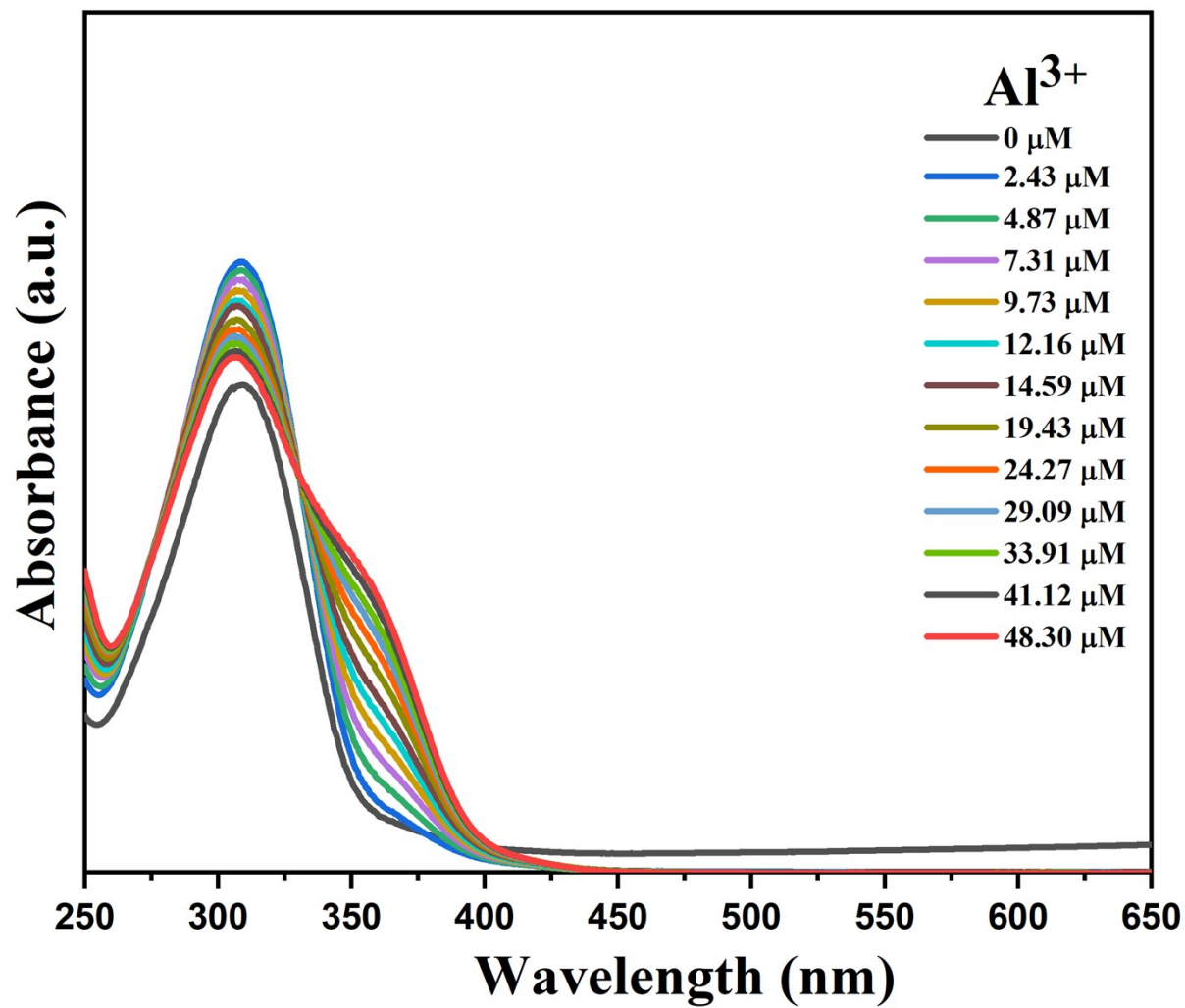


Fig. S42: Absorption spectra of **1** dispersed in water upon incremental addition of water solution of Al³⁺ ions. Final concentration of Al³⁺ ions in the medium is indicated in the legend.

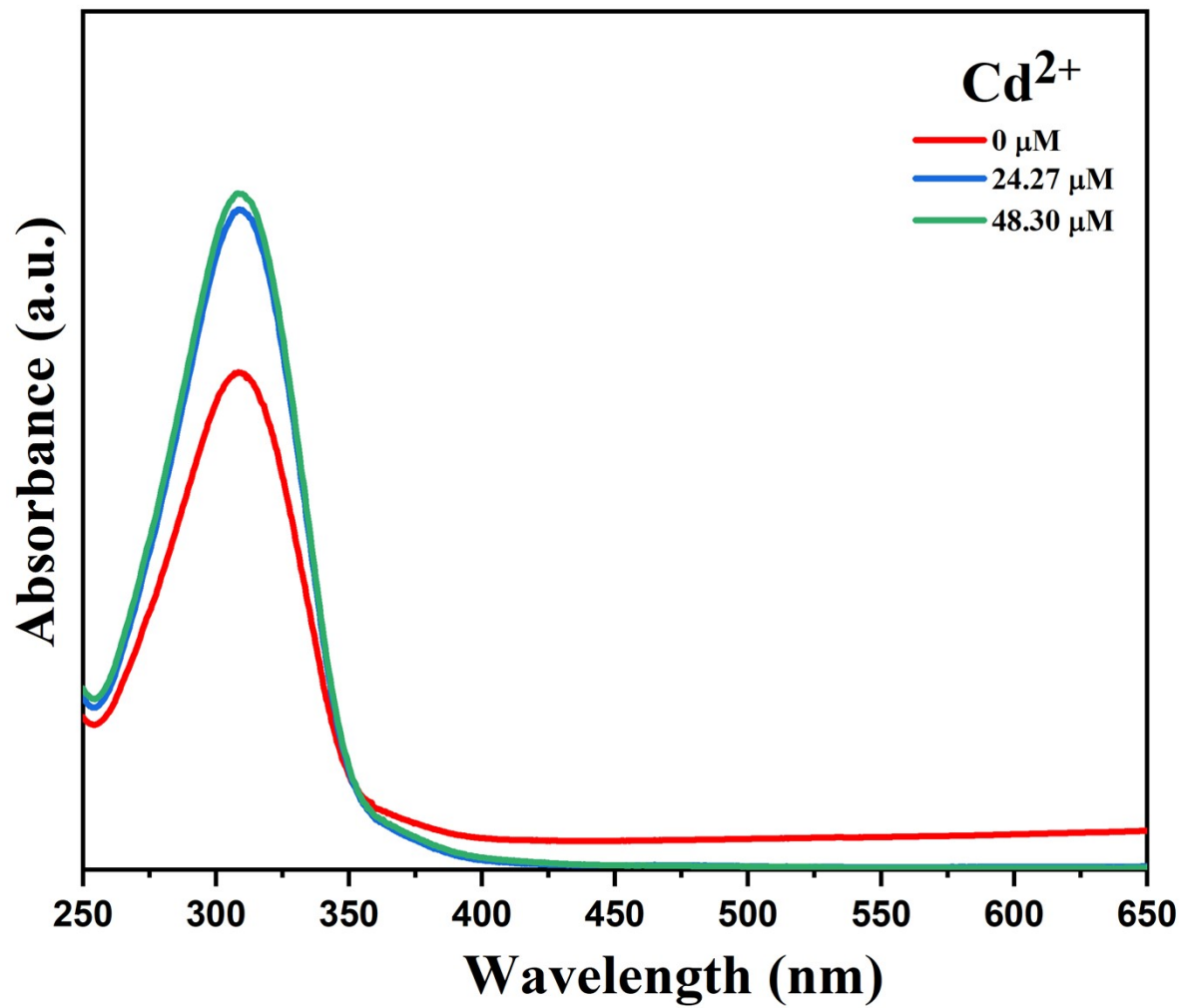


Fig. S43: Absorption spectra of **1** dispersed in water upon incremental addition of water solution of Cd²⁺ ions. Final concentration of Cd²⁺ ions in the medium is indicated in the legend.

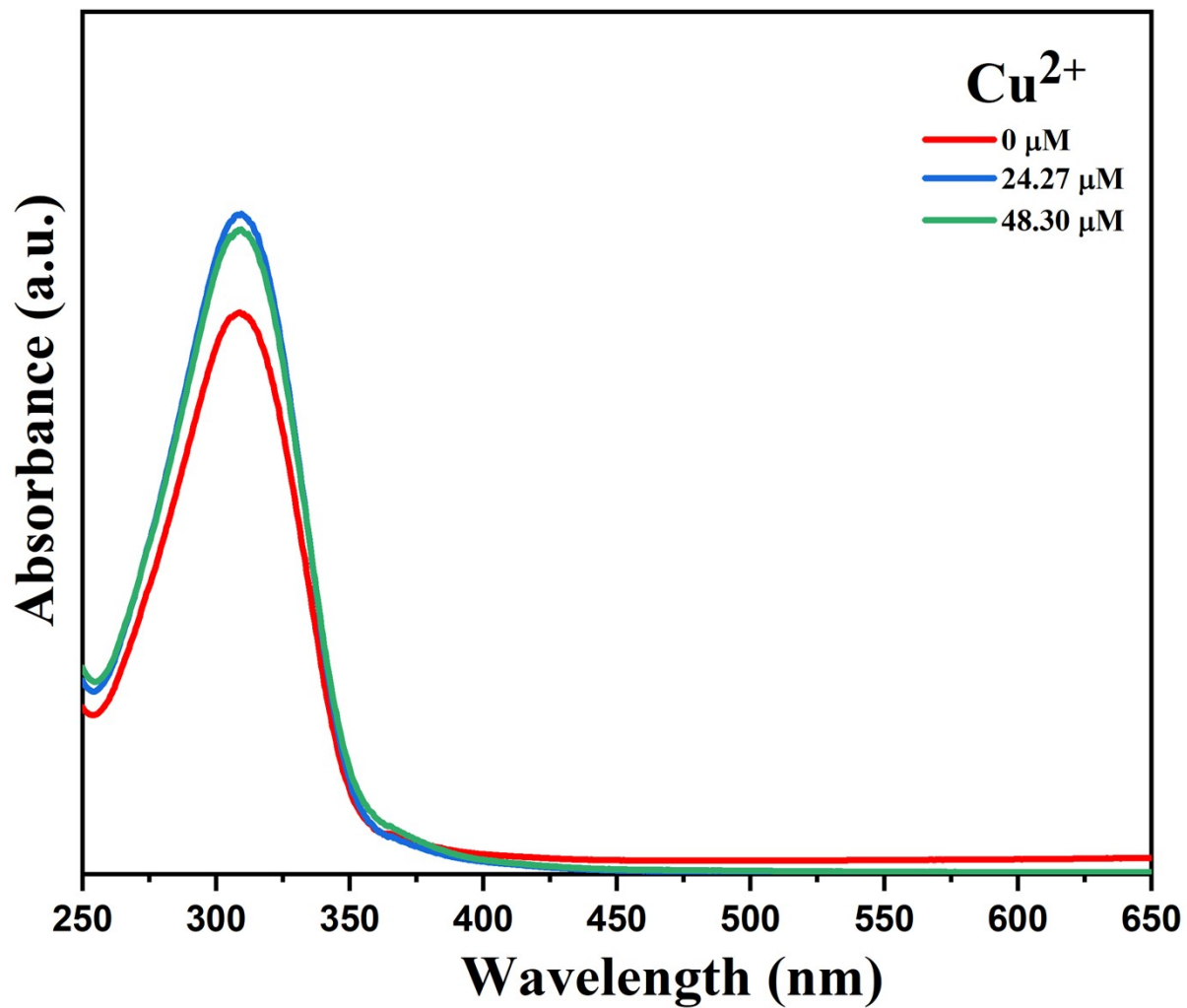


Fig. S44: Absorption spectra of 1 dispersed in water upon incremental addition of water solution of Cu²⁺ ions. Final concentration of Cu²⁺ ions in the medium is indicated in the legend.

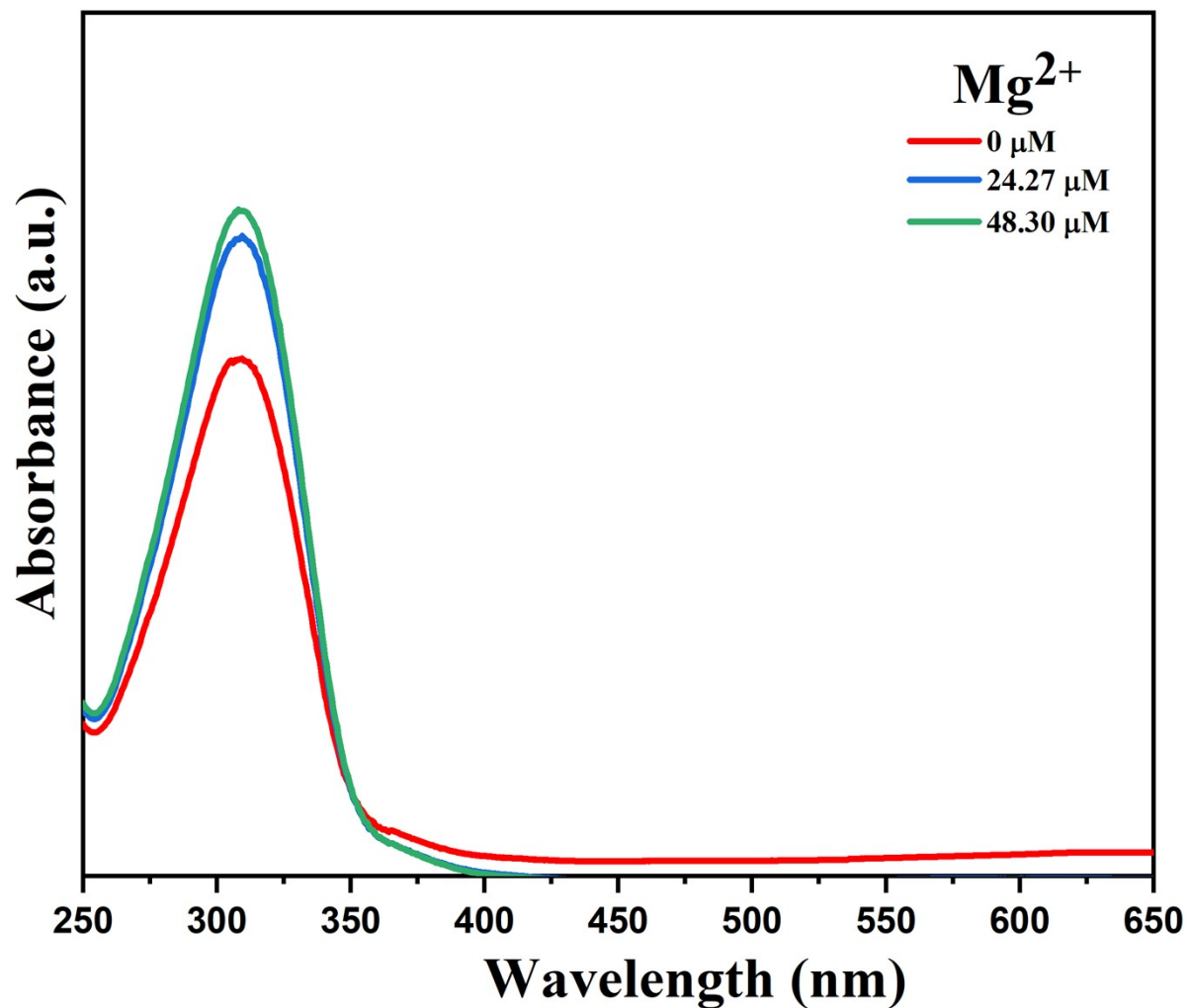


Fig. S45: Absorption spectra of **1** dispersed in water upon incremental addition of water solution of Mg²⁺ ions. Final concentration of Mg²⁺ ions in the medium is indicated in the legend.

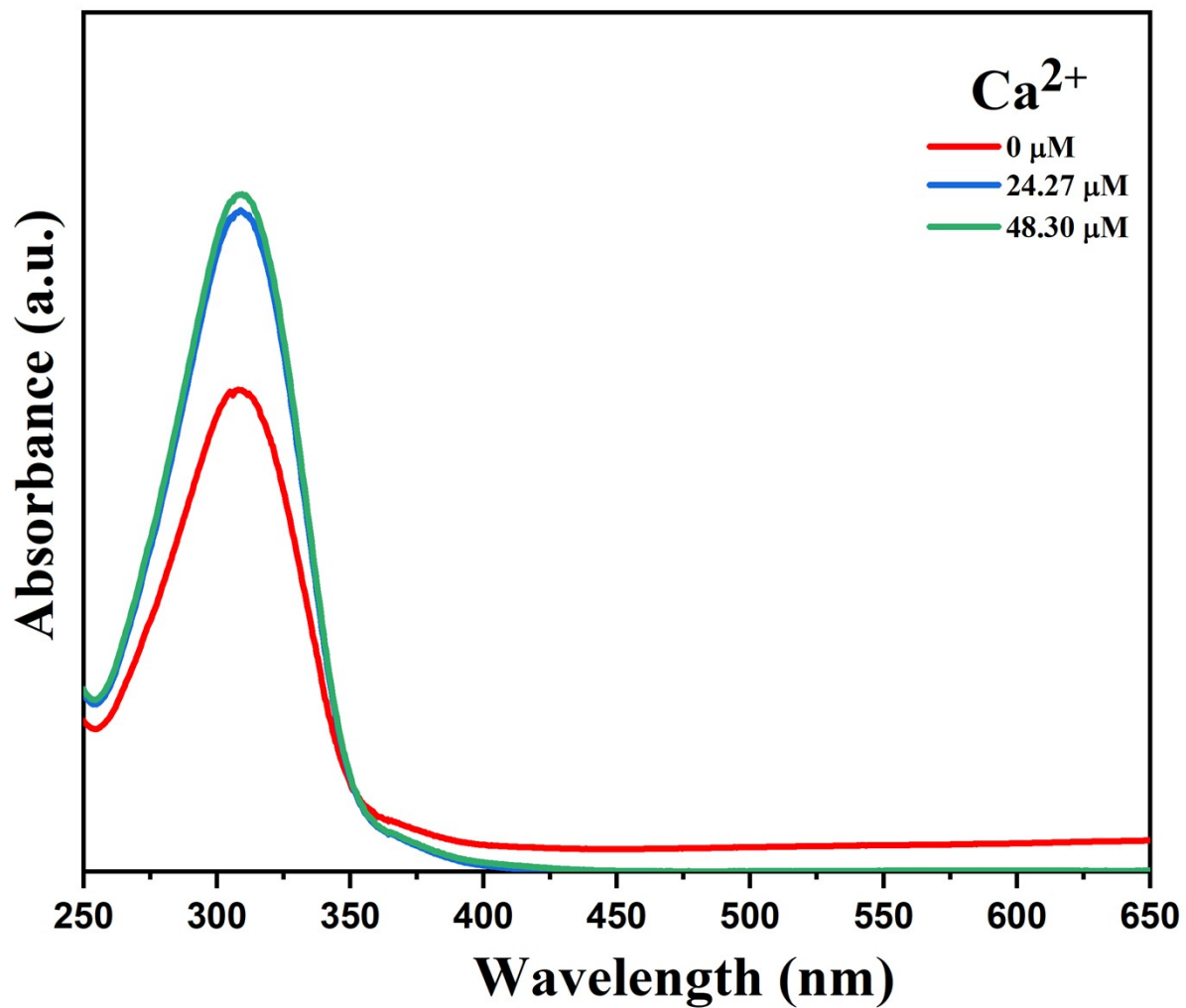


Fig. S46: Absorption spectra of **1** dispersed in water upon incremental addition of water solution of Ca²⁺ ions. Final concentration of Ca²⁺ ions in the medium is indicated in the legend.

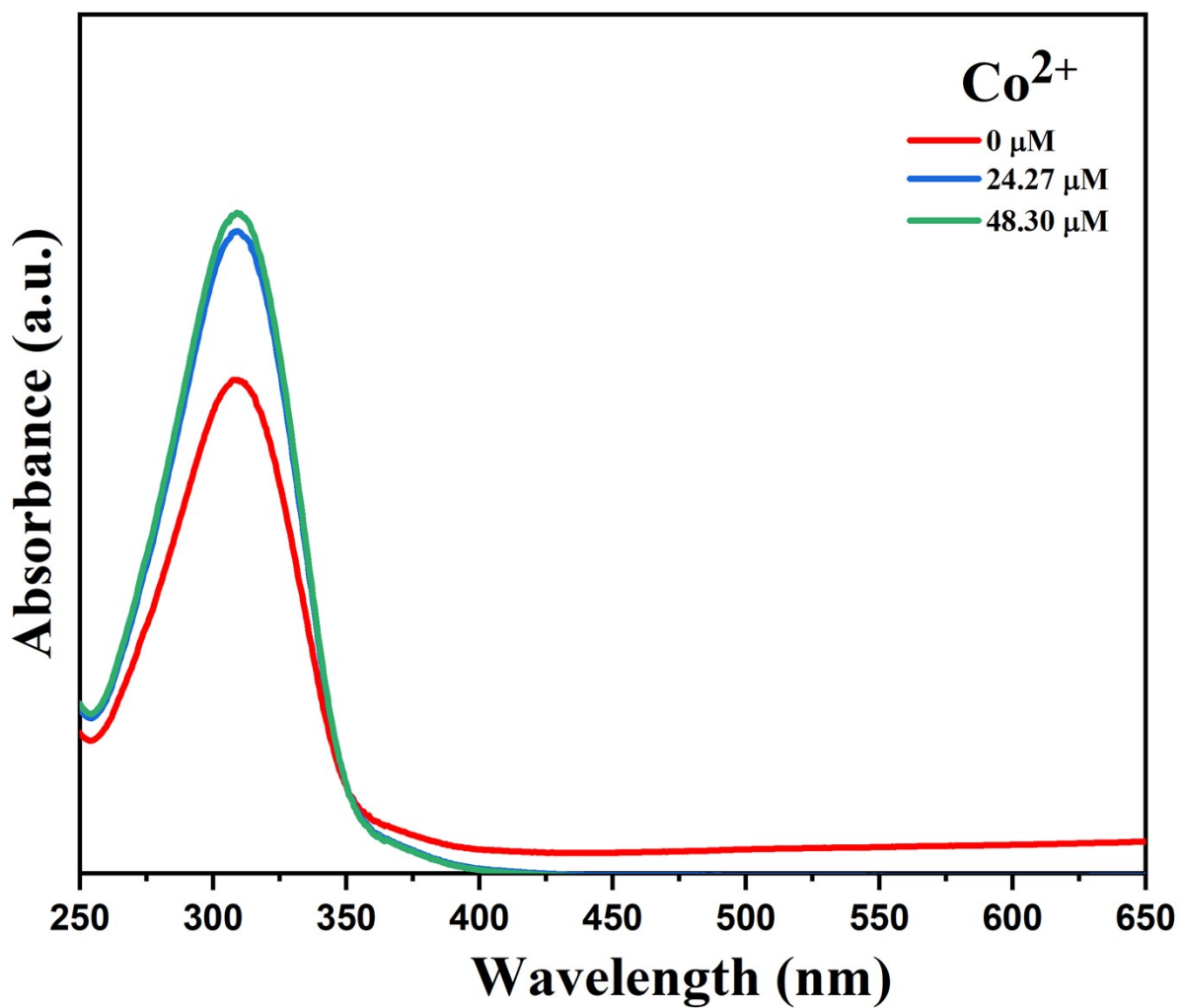


Fig. S47: Absorption spectra of **1** dispersed in water upon incremental addition of water solution of Co^{2+} ions. Final concentration of Co^{2+} ions in the medium is indicated in the legend.

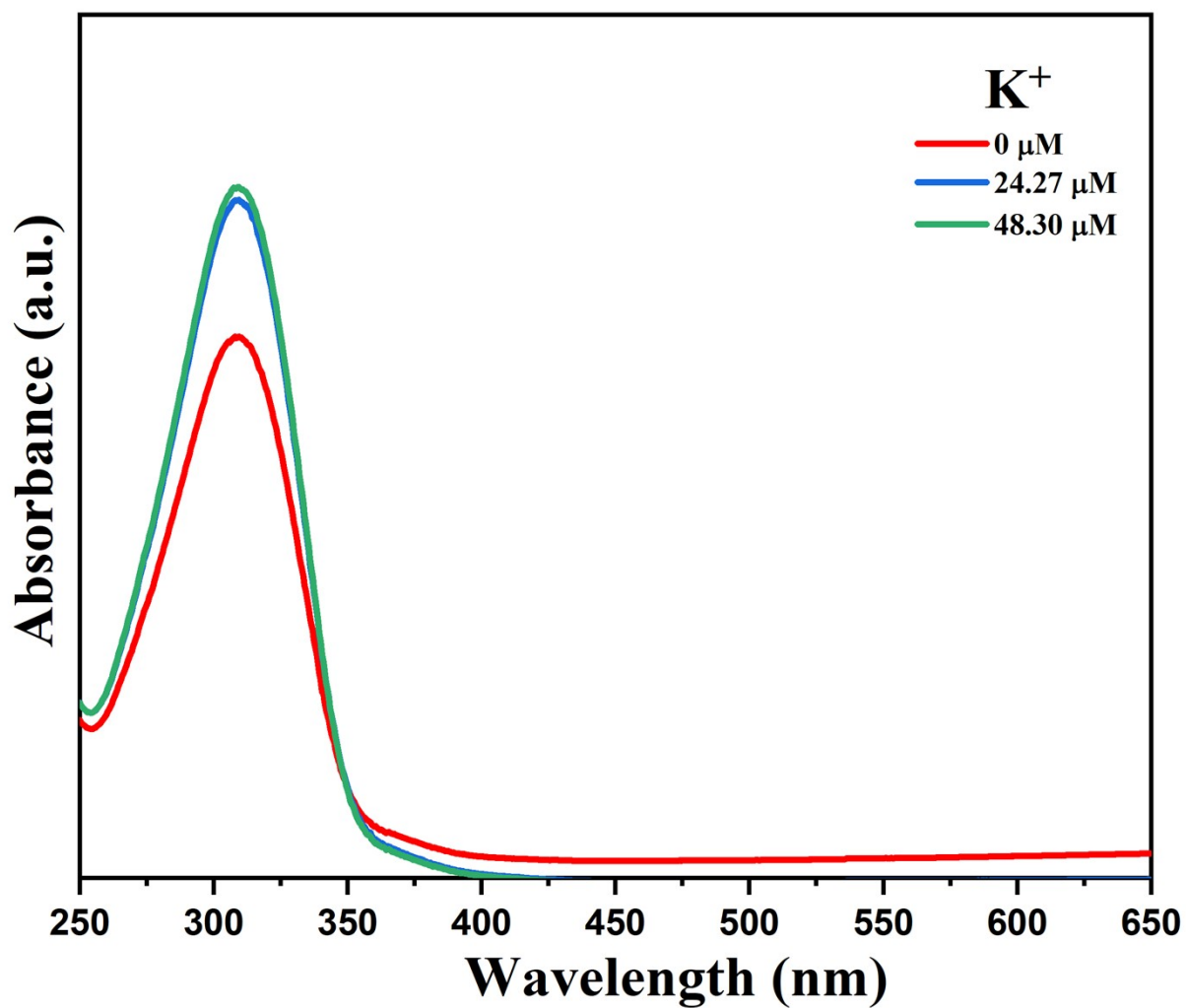


Fig. S48: Absorption spectra of **1** dispersed in water upon incremental addition of water solution of K⁺ ions. Final concentration of K⁺ ions in the medium is indicated in the legend.

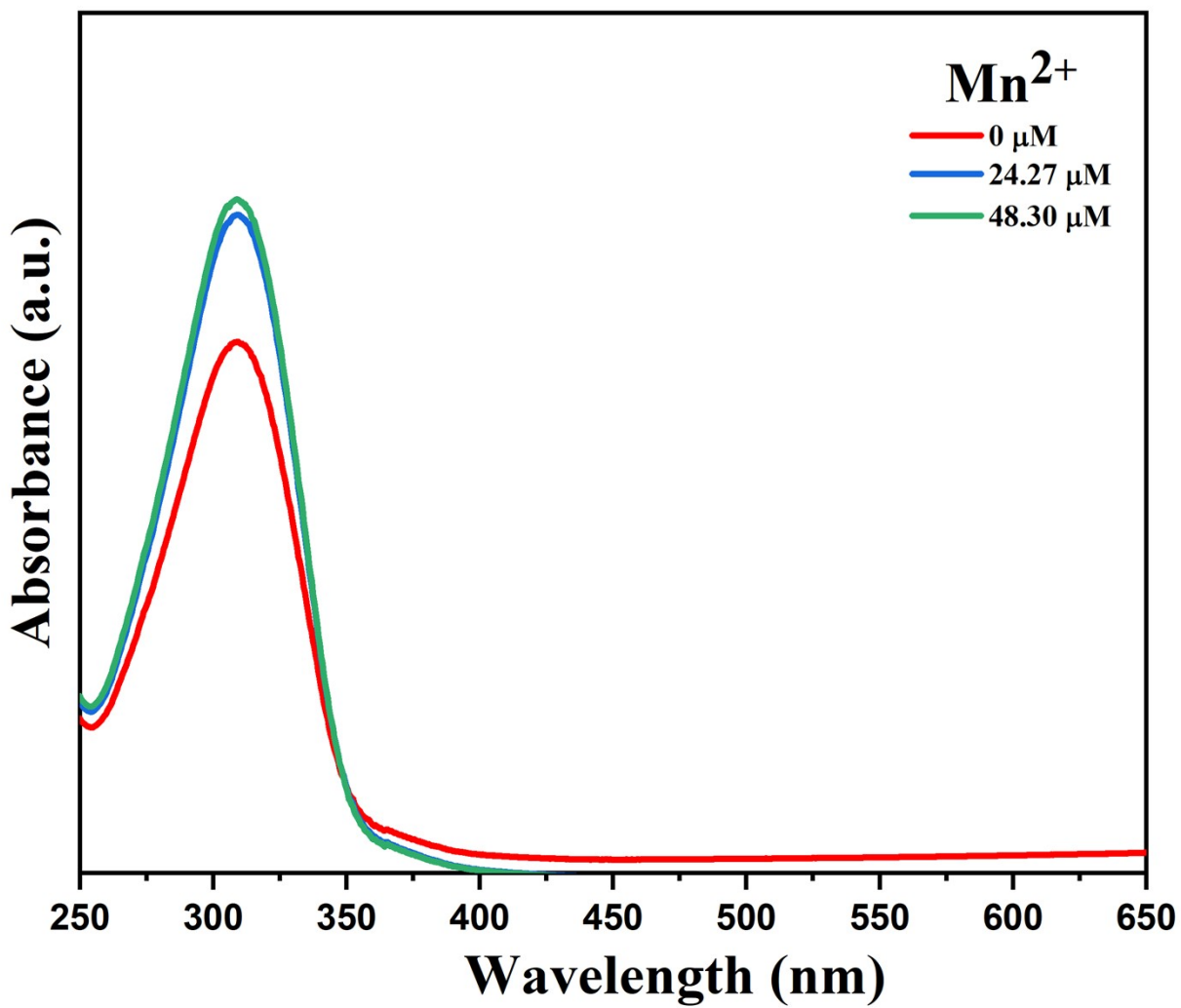


Fig. S49: Absorption spectra of **1** dispersed in water upon incremental addition of water solution of Mn²⁺ ions. Final concentration of Mn²⁺ ions in the medium is indicated in the legend.

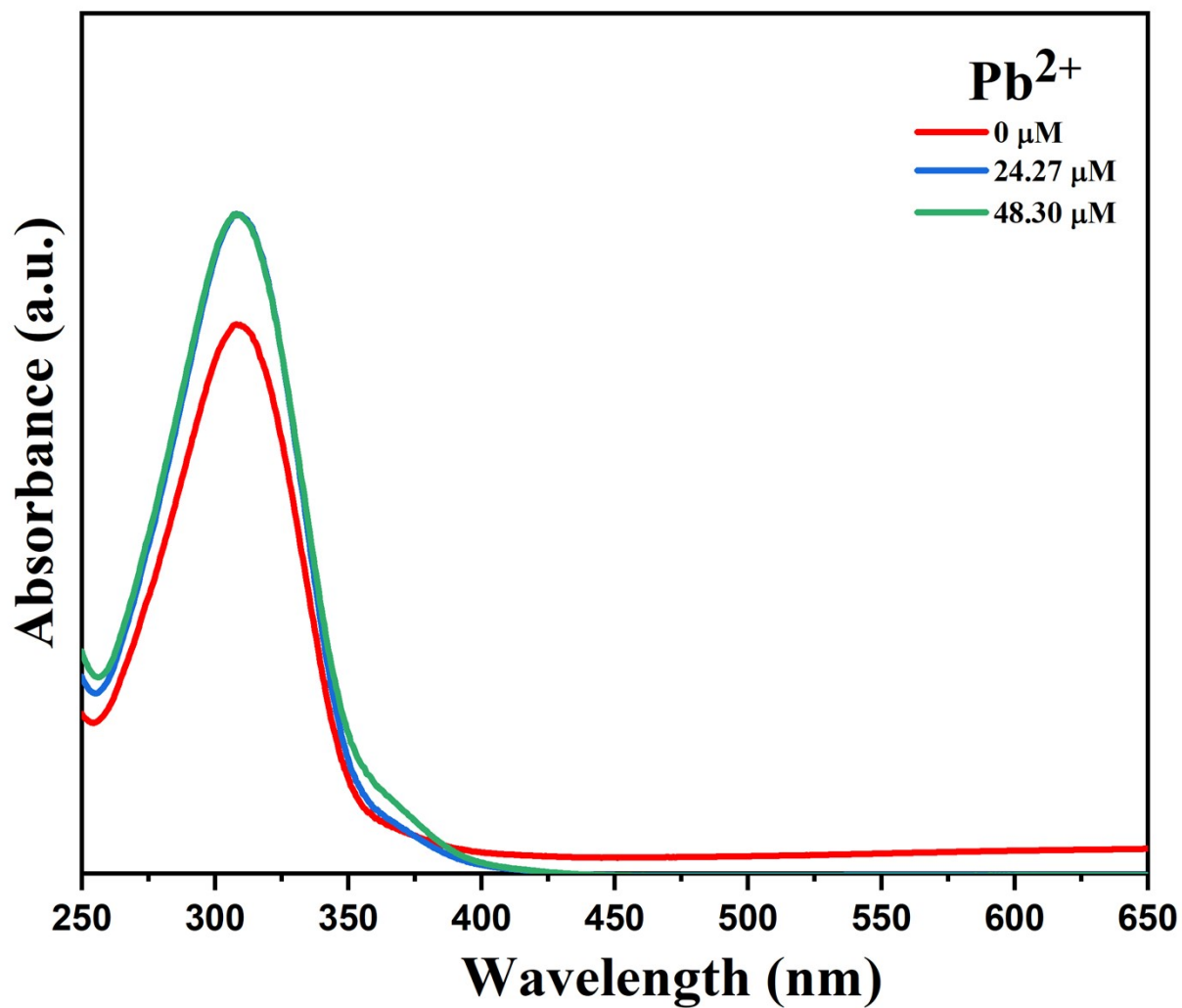


Fig. S50: Absorption spectra of 1 dispersed in water upon incremental addition of water solution of Pb^{2+} ions. Final concentration of Pb^{2+} ions in the medium is indicated in the legend.

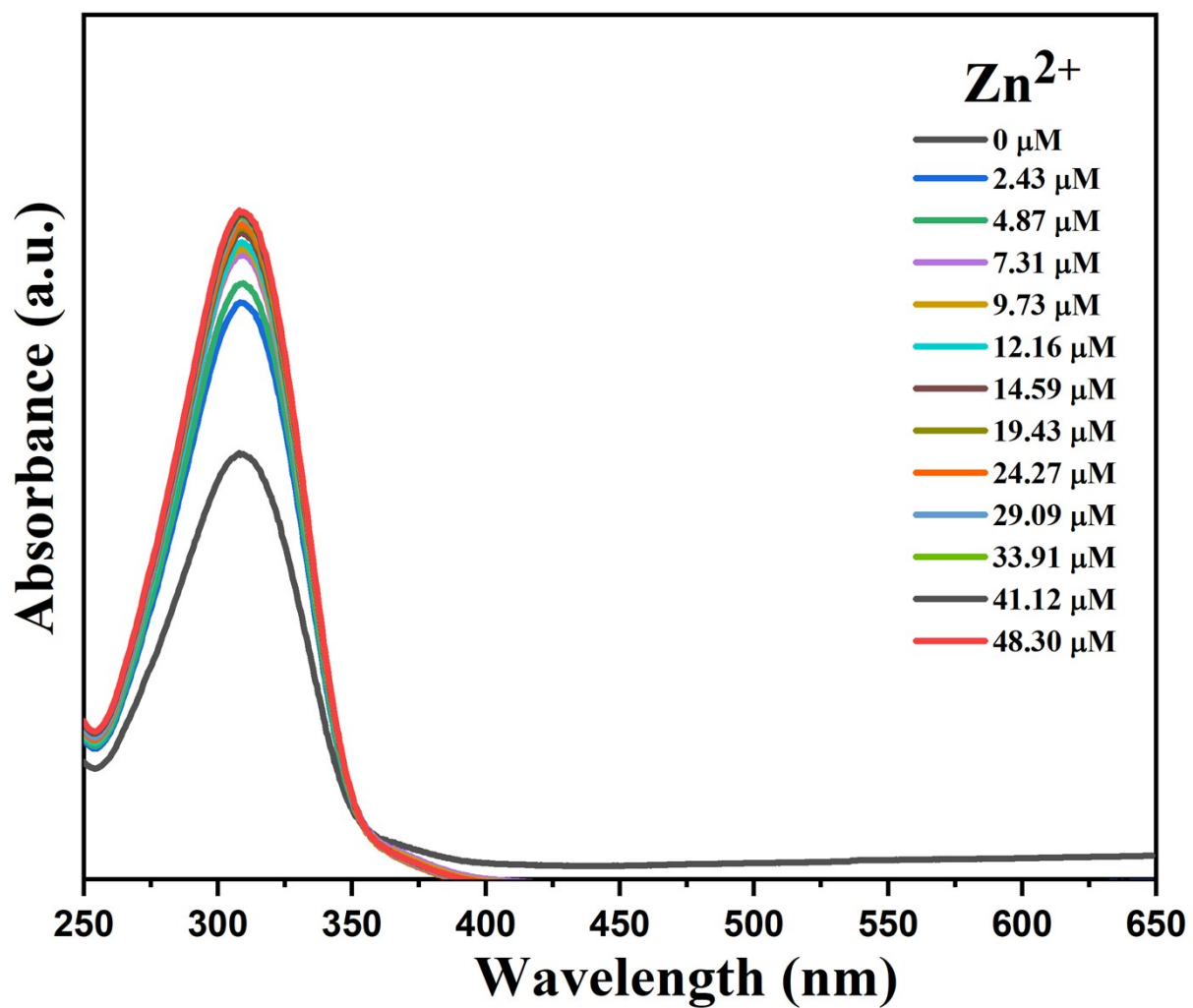


Fig. S51: Absorption spectra of 1 dispersed in water upon incremental addition of water solution of Zn²⁺ ions. Final concentration of Zn²⁺ ions in the medium is indicated in the legend.

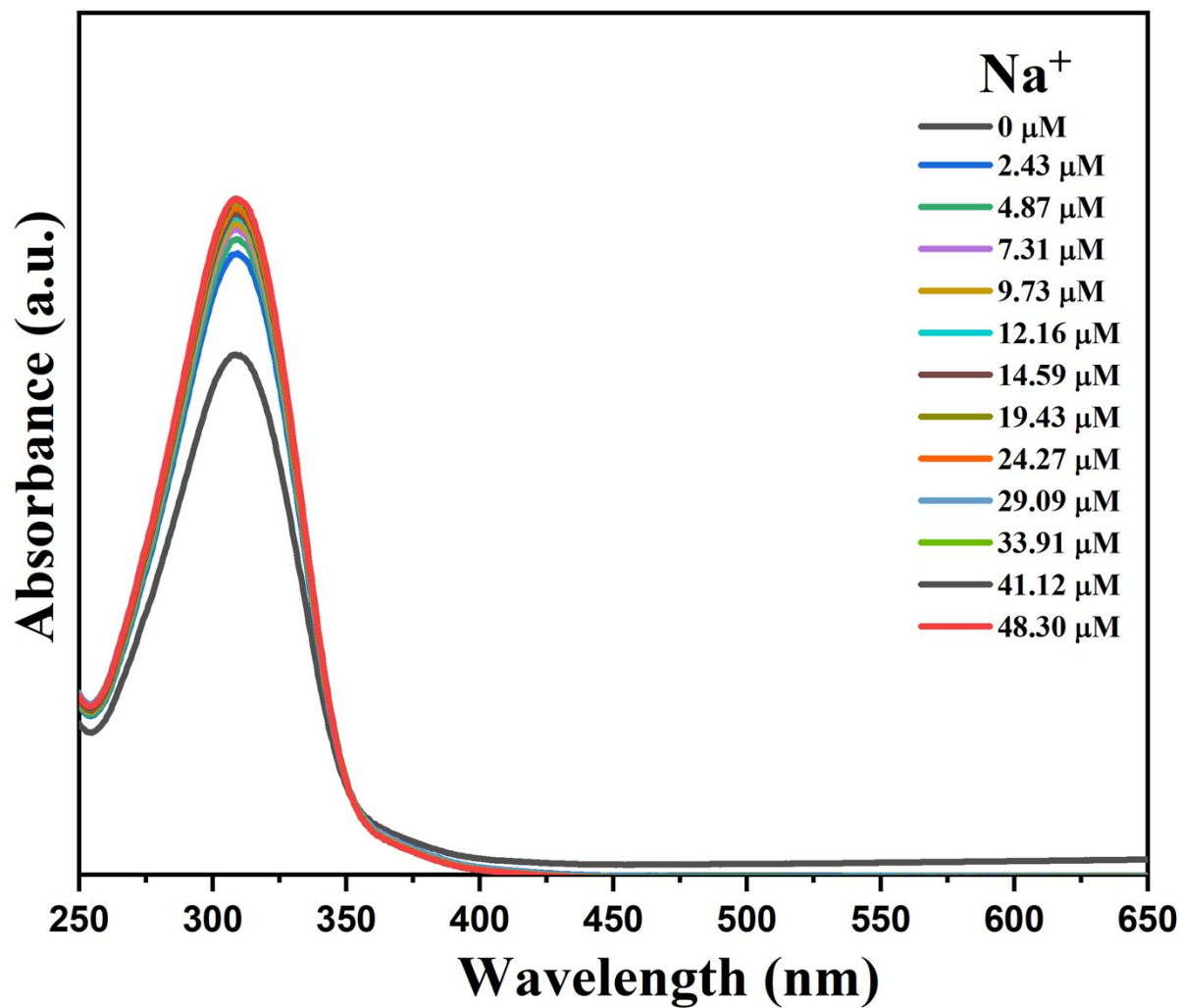


Fig. S52: Absorption spectra of 1 dispersed in water upon incremental addition of water solution of Na⁺ ions. Final concentration of Na⁺ ions in the medium is indicated in the legend.

Table S6: A summary of luminescence-based sensing of Fe³⁺ ion using MOFs.

MOF	Medium	LOD (μM)	K_{sv} (M^{-1})	Ref.
$\{[\text{Cd}_2(\text{SA})_2(\text{L})_2] \cdot \text{H}_2\text{O}\}_n$	DMF	2.4	2.1×10^4	89
$[\text{Cd}_2(\text{OBA})_2(\text{BPTP})(\text{H}_2\text{O})]$	DMF	0.36	—	90
$[\text{Zn}(5\text{-AIP})(\text{Ald-4})] \cdot \text{H}_2\text{O}$	H ₂ O	0.30	9.00×10^4	91.
$[\text{Zn}(\text{L})(\text{bpdc})] \cdot 1.6\text{H}_2\text{O}$	DMF	5.62	1.73×10^4	92
$[\text{Cd}(\text{H}_2\text{BDDBA})]_n$	H ₂ O	—	8.79×10^4	93
$[\text{Cd}(\text{PAM})(4\text{-bpdb})_{1.5}] \cdot \text{DMF}$	H ₂ O	0.3	3.5×10^4	94
$[\text{Cu}(\text{tpp}) \cdot \text{H}_2\text{O}]_{2n}$	H ₂ O	10	4.6×10^4	95
$\{[\text{Cd}_3(\text{L}^{2-})_3(\text{H}_2\text{O})] \cdot (\text{DMF}) \cdot (\text{H}_2\text{O})\}_n$	DMF	—	2.07×10^4	96
$[\text{Zn}_2(\text{oba})_2(\text{bpy})]$	MeOH	0.3	5.8×10^4	97
Ag-MOFs(1–3)	H ₂ O	11.46, 15.83, 15.44	(0.936, 1.033, and $0.888) \times 10^4$	98
JXUST-18	EtOH	0.196	—	99
$[\text{Cd}(\text{PDA})(\text{L})_2]$	H ₂ O	1.34	23.29×10^4	This work

Table S7: A summary of luminescence-based sensing of Cr³⁺ ions using MOFs.

MOF	Medium	LOD (μM)	K_{sv} (M^{-1})	Ref.
[Zn (tbda)] _n	H ₂ O	180	2.68×10^3	100
[Eu ₂ (tpbpc) ₄ ·CO ₃ ·4H ₂ O]·DMF·solvent	H ₂ O	68.8	5.14×10^2	101
{[Zn(H ₂ dhbdc)(bpycz)]·0.5H ₂ O} _n	H ₂ O	8.22	4.85×10^3	102
[Zn(Br-1,4-bdc) (bpycz)] _n	H ₂ O	4.73	4.04×10^3	102
{[Zn(tta) _{0.5} (m-bimb)]·H ₂ O} _n	DMF	—	0.65	103
[Zn ₂ (TPOM)(NH ₂ -BDC) ₂]·4H ₂ O	DMF	4.9	—	52
[Zn(L)(H ₂ O)]·H ₂ O	H ₂ O	2.44	2.03×10^4	104
[Zn(5-AIP)(Ald-4)]·H ₂ O	H ₂ O	0.46	2.30×10^4	91
{[Zn(BIBT)(oba)]·DMA} _n	EtOH	0.049	—	105
[Me ₂ NH ₂] ₄ [Zn ₆ (qptc) ₃ (trz) ₄]·6H ₂ O	H ₂ O	1	4.39×10^4	106
Zn ₃ (bpdc) ₂ (pdc)(DMF)·6DMF	DMF	25.1	3870	107
[Cd(PDA)(L) ₂]	H ₂ O	4.95	5.06×10^4	This work

Table S8: A summary of luminescence-based sensing of Al³⁺ ions using MOFs.

MOF	Medium	LOD (μM)	K _{sv} (M^{-1})	Ref.
$\{[\text{Zn}_2(\text{O-BTC})(4,4'\text{-BPY})_{0.5}(\text{H}_2\text{O})_3] \cdot (\text{H}_2\text{O})_{1.5} \cdot (\text{DMA})_{0.5}\}_n$	EtOH	3.70	—	59
$[\text{Zn}(\text{DMA})(\text{TBA})]$	H ₂ O	1.97	1.33×10^4	108
$[\text{Co}_2(\text{dmimpym})(\text{nda})_2]_n$	DMF	0.7	—	109
$\{[\text{Cd}(\text{CDC})(\text{L})]\}_n$	DMF	61	2.6×10^3	89
$[\text{Cd}(\text{L})(\text{phen})_2] \cdot 5\text{H}_2\text{O}$	DMF	0.113	2.49×10^4	110
HPU-24@Ru	H ₂ O	11.63	—	111
$\{[\text{Co}(\text{L})(\text{bibp})]\}_n$	H ₂ O	1.52	1.97×10^4	112
$[\text{Zn}(5\text{-AIP})(\text{Ald-4})] \cdot \text{H}_2\text{O}$	H ₂ O	0.35	2.80×10^4	91
$[\text{Cd}(\text{PAM})(4\text{-bpdb})_{1.5}] \cdot \text{DMF}$	H ₂ O	0.56	2.3×10^4	113
$\{[\text{Cd}_2(\text{SA})_2(\text{L})_2] \cdot \text{H}_2\text{O}\}_n$	DMF	93	5.4×10^3	89
$[\text{Co}(\text{OBA})(\text{DATZ})_{0.5}(\text{H}_2\text{O})]$	H ₂ O	2.5	—	114
$[\text{Cd}(\text{PDA})(\text{L})_2]$	H ₂ O	3.96	3.09×10^4	This work

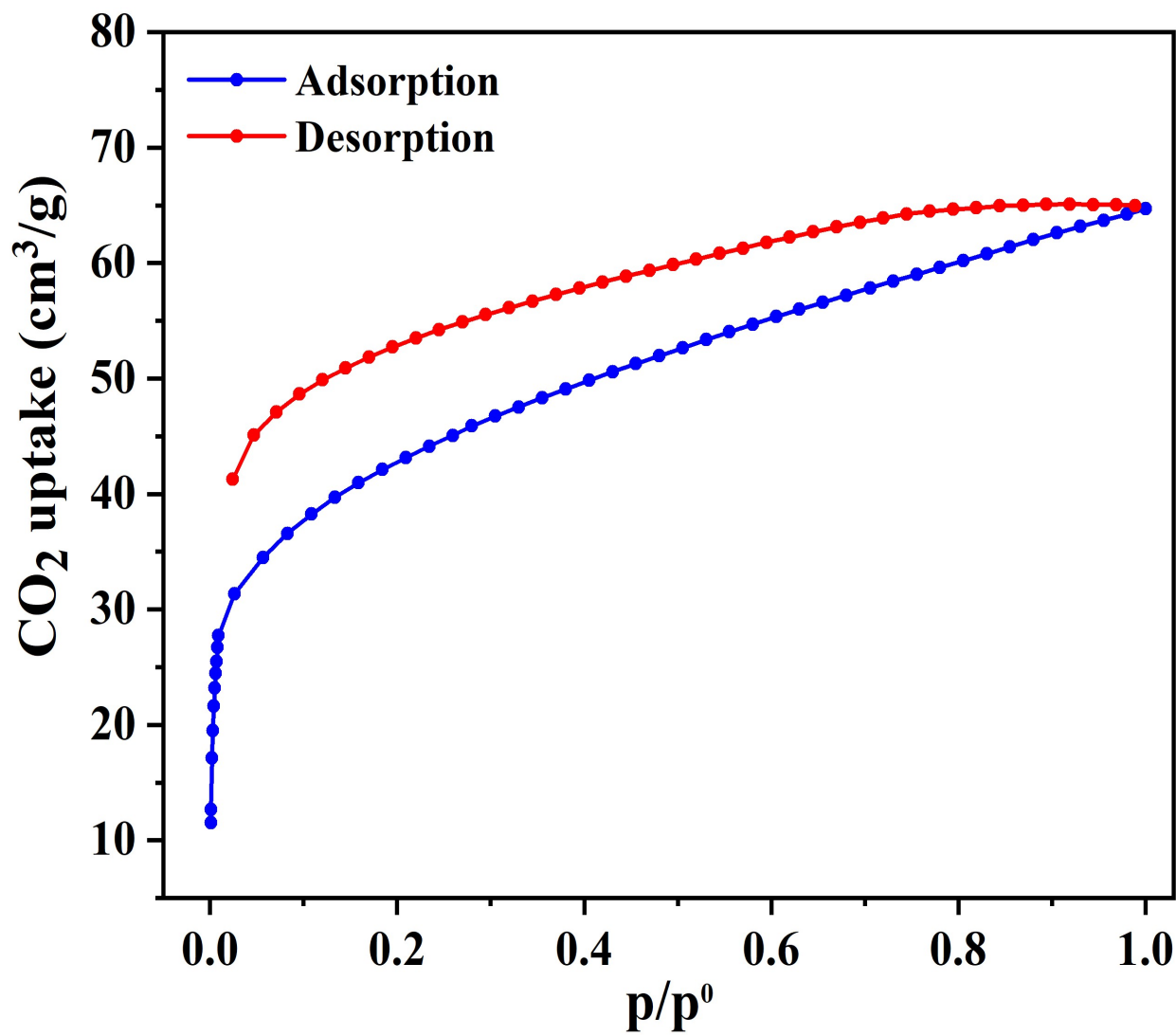


Fig. S53: CO₂ gas sorption isotherm of 1 at 195 K.

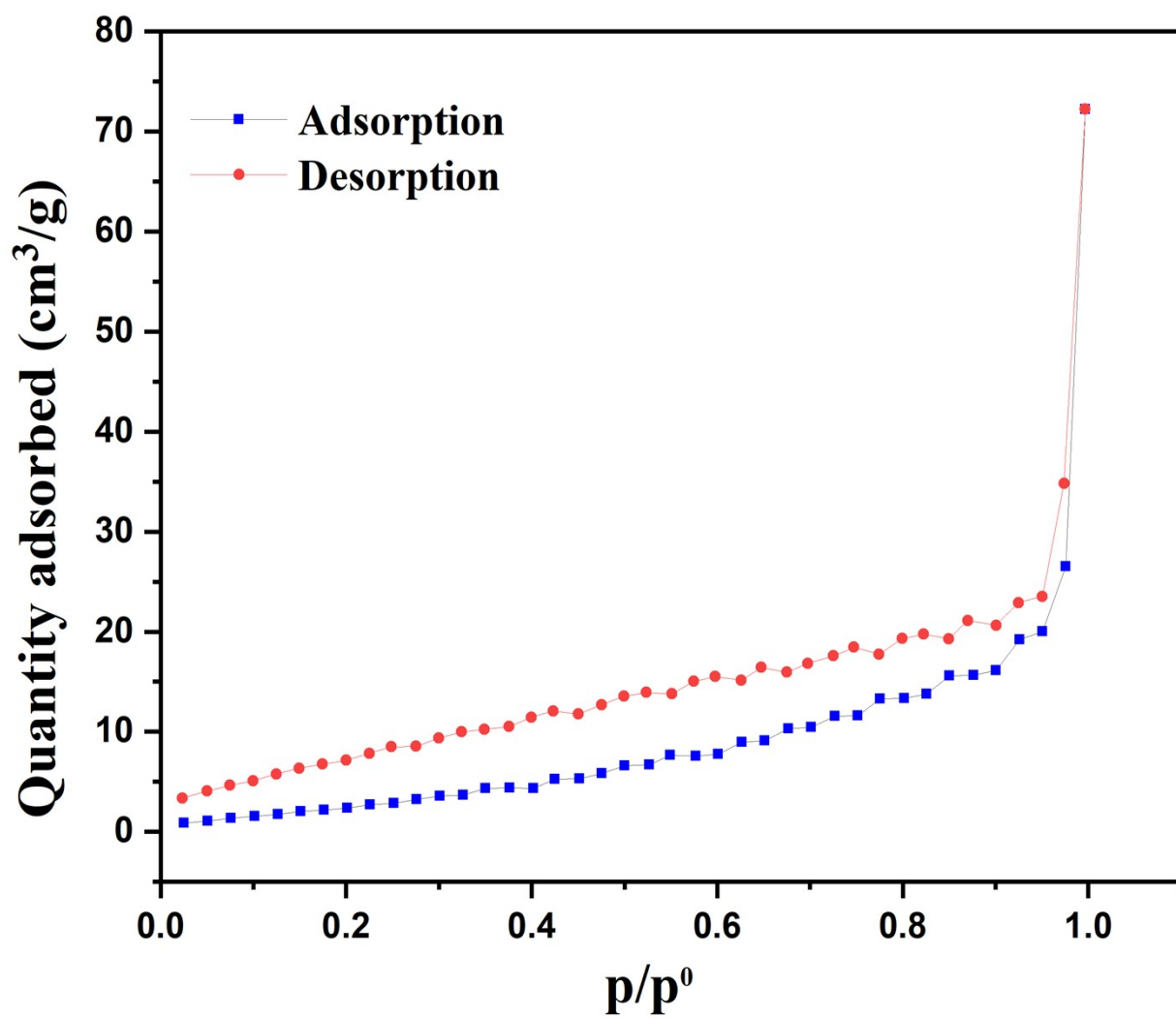


Fig. S54: N₂ gas sorption isotherm of 1 at 77 K.

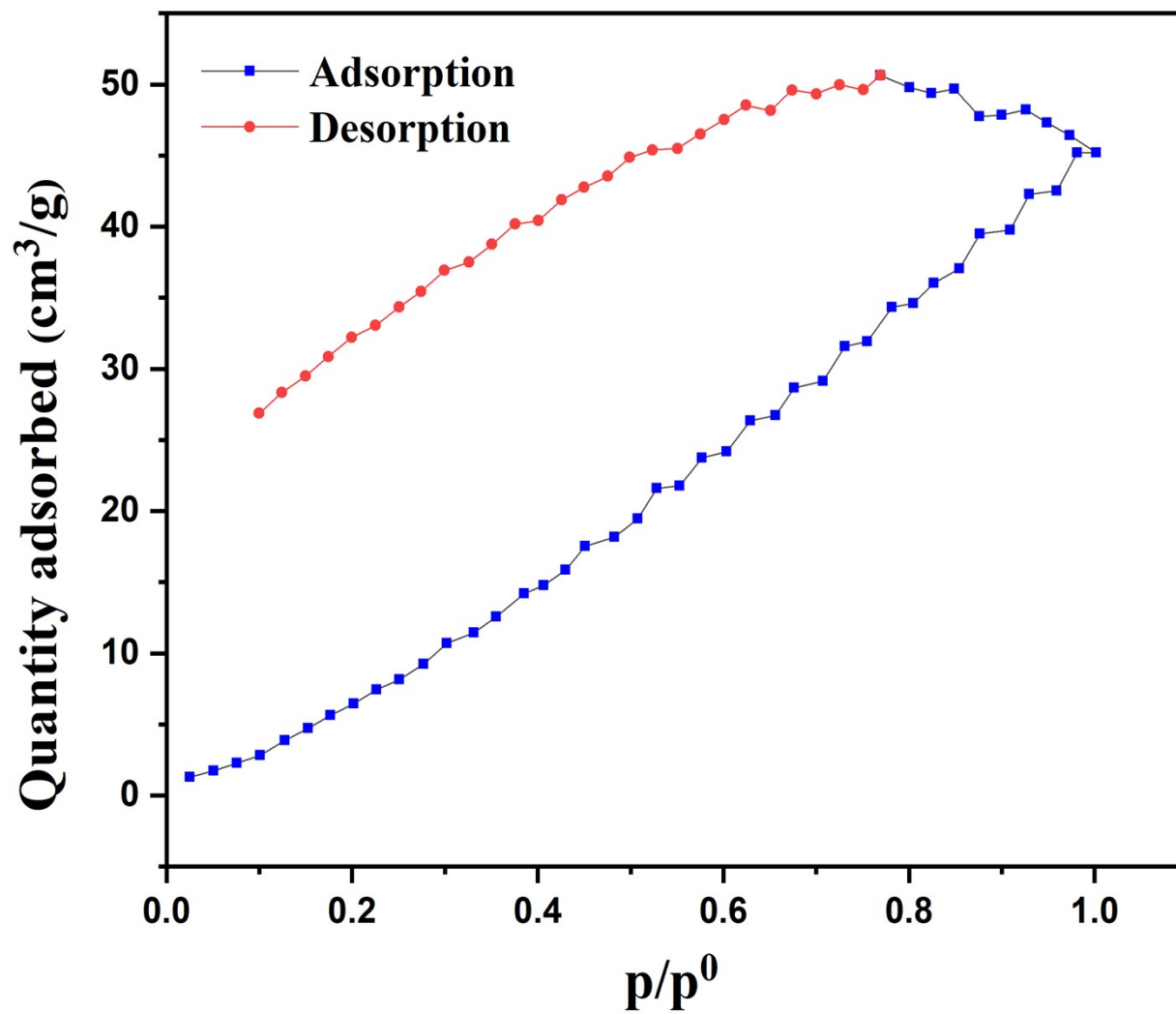


Fig. S55: H₂ gas sorption isotherm of **1** at 77 K.

Table S9: A summary of CO₂ gas adsorption using MOFs.

MOFs	Surface area from N ₂ adsorption [m ² g ⁻¹]	CO ₂ uptake cm ³ /g at 195 K	Ref.
$\{[\text{Cd}_2(\text{sdb})_2(4\text{-bpmh})_2(\text{H}_2\text{O})]\}_n \cdot 2n(\text{H}_2\text{O})$	—	39.19	115
$\{[\text{Cd}_2(\text{sdb})_2(3\text{-bpmh})_2]\}_n \cdot 3n(\text{H}_2\text{O}) \cdot n(\text{C}_6\text{H}_5\text{NO})$	—	60.9	115
$[\text{Mg}_{16}(\text{PTCA})_8(\mu_2\text{-H}_2\text{O})_8(\text{H}_2\text{O})_{16}(\text{dioxane})_8] \cdot (\text{H}_2\text{O})_{13} \cdot (\text{DMF})_{26}$	438.1	160.5	116
$\{[\text{Zn}(\text{H}_2\text{dhdcb})_2(\text{bpycz})] \cdot 0.5\text{H}_2\text{O}\}_n$	291.4	101.1	102
$[\text{Zn}(\text{Br-1,4-bdc})(\text{bpycz})]_n$	288.5	98.6	102
Cu-MOF	945	201.6	117
$[\text{Cu}_3(3,3'\text{-dmglut})_3(\text{bte})] \cdot 6(\text{H}_2\text{O})\}_n$ and $[\text{Cu}(3,3'\text{-dmglut})(\text{btp})_{0.5}] \cdot 2(\text{H}_2\text{O})\}_n$	—	21 and 26.2	118
Cu-MOP	270.9	96.5	119
ZnDatzBdc	303	92.5	120
$[\text{Cd}(\text{PDA})(\text{L})_2]$	11.635	64.5	This work