Supplementary Information

A Novel Multimode Sensor Showing Cation-Dependent Fluorescence Colour

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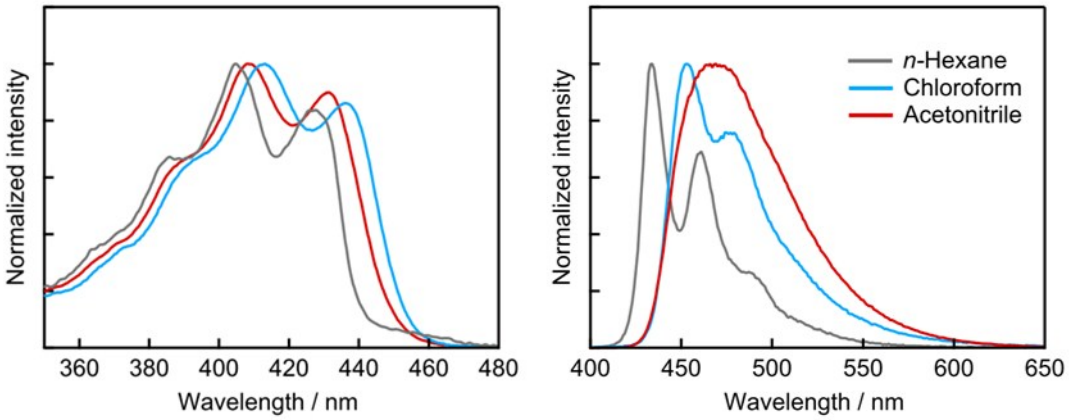

Figure S1. Absorption (left) and fluorescence (right) spectra of compound **1** in *n*-hexane (ε_r = 2.0), chloroform (4.8), and acetonitrile (37). ε_r is the dielectric constant of the solvent.

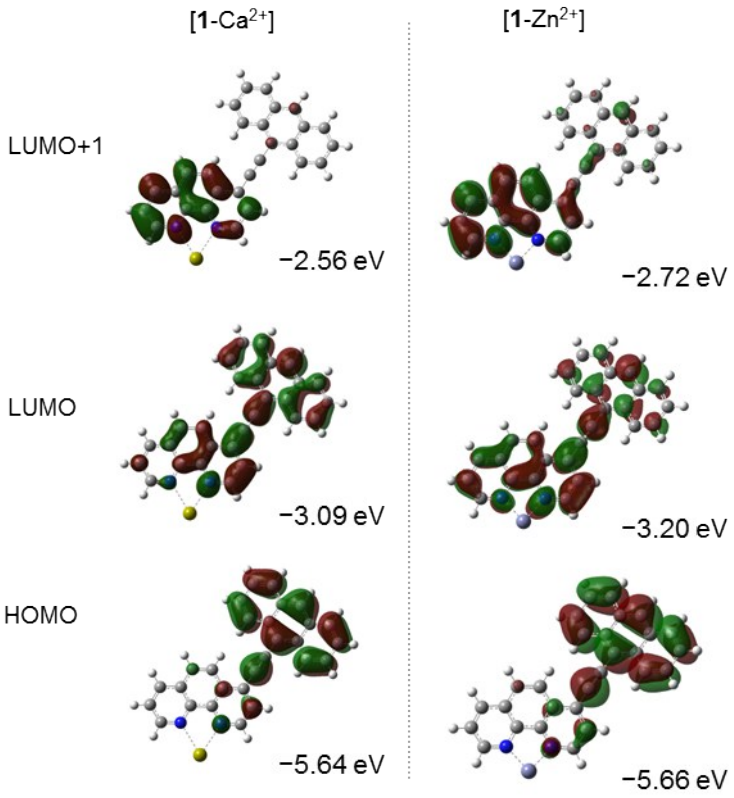

Figure S2. Electron densities in the HOMO, LUMO, and LUMO+1 levels of the [**1**-Ca^{2+}] and [**1**-Zn^{2+}] complexes evaluated by DFT calculations (B3LYP/6-31G(d, p)).

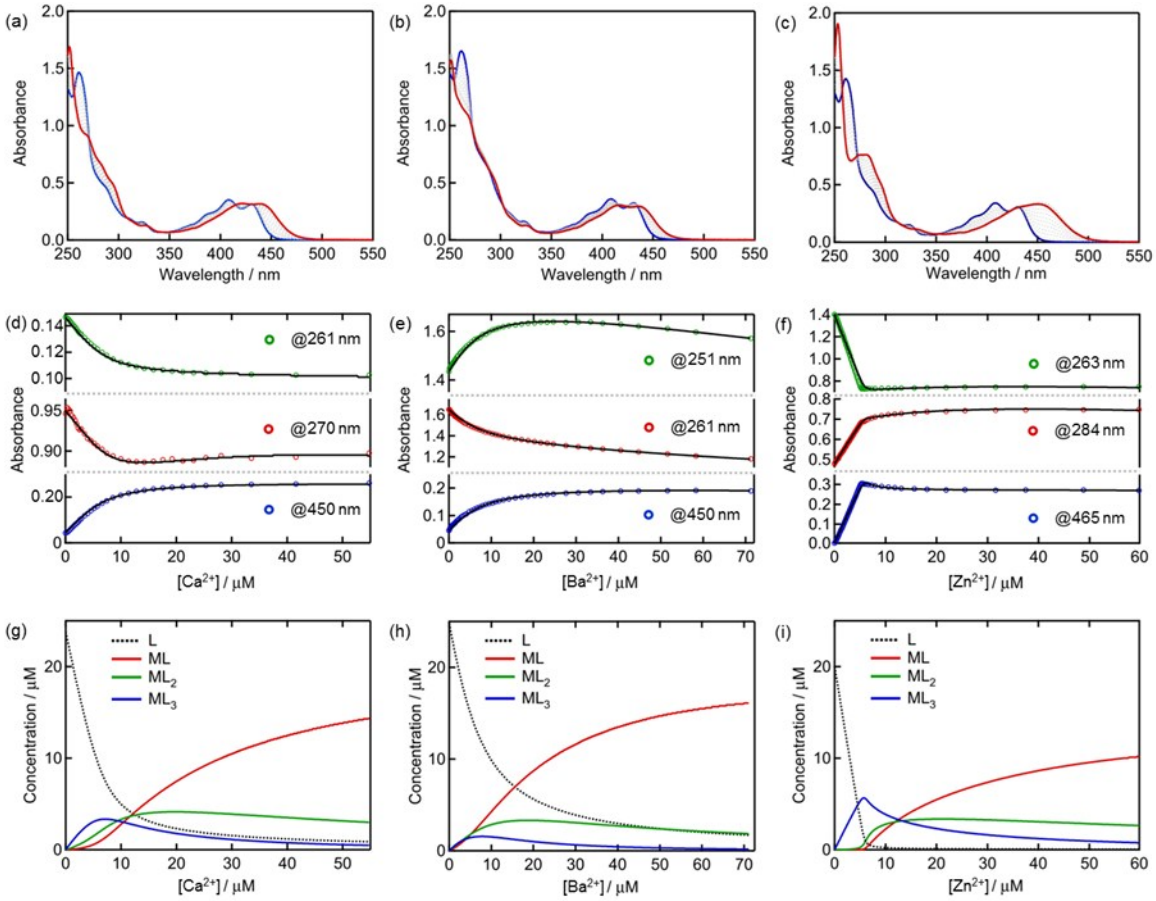

Figure S3. (a, b, c) UV-vis absorption spectra of **1** upon titration by (a) Ca^{2+} ([**1**] = 2.4 x 10^{-6} M), (b) Ba^{2+} ([**1**] = 2.5 x 10^{-6} M), and (c) Zn^{2+} ([**1**] = 2.0 x 10^{-6} M) in acetonitrile. The blue and red curves show the spectra of **1** before and after ((6.0 ~ 7.0) x 10^{-6} M) an addition of M^{2+}, respectively. (d, e, f) Titration curves monitored at several wavelengths (open circles) and their simulated curves (solid curves). (g, h, i) Concentration changes of [L], [ML], [ML_2], and [ML_3] during titration evaluated by spectral analysis.

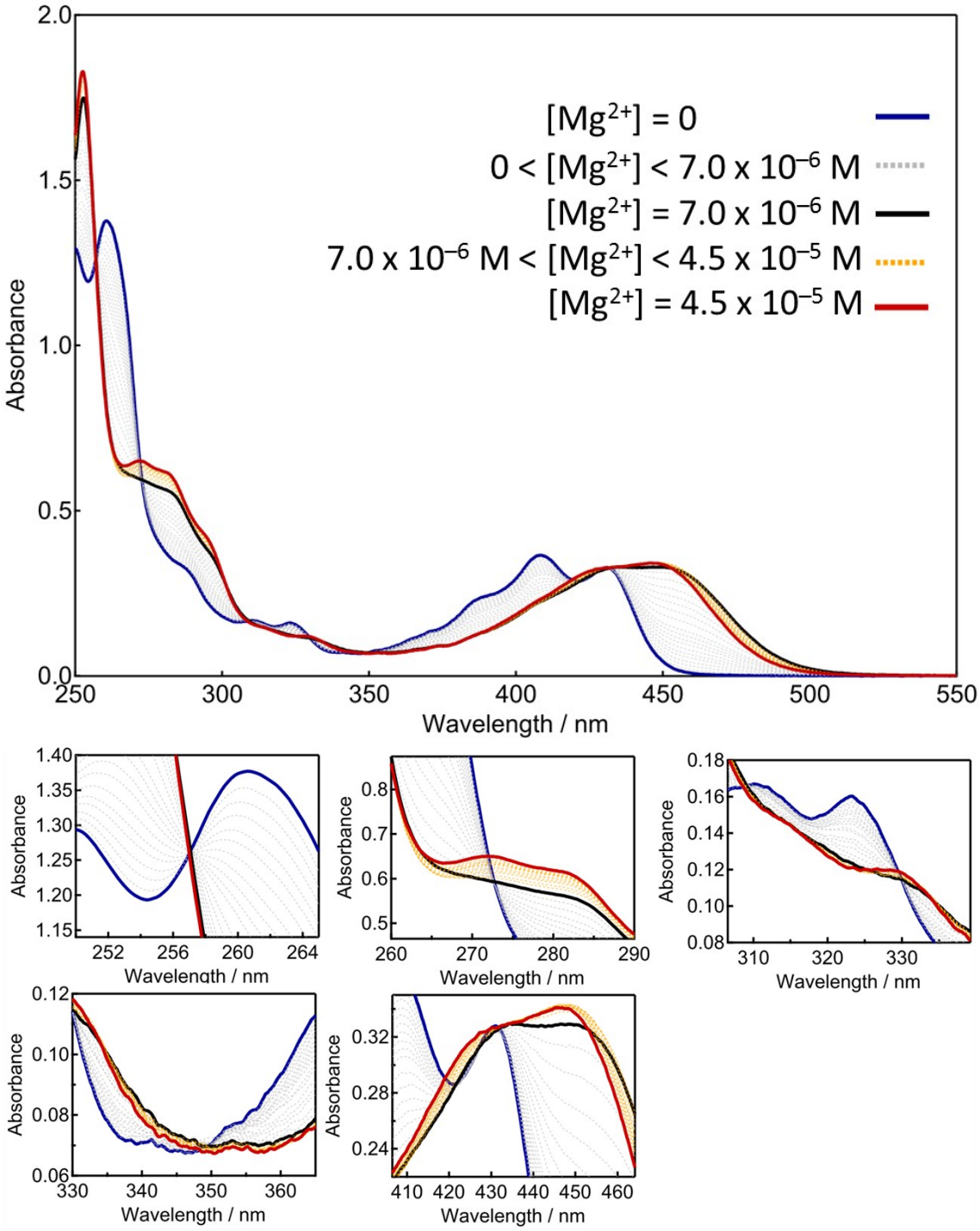

Figure S4. Enlarged view of Fig.2a: UV-vis absorption spectra of **1** (2.1 x 10^{-6} M) upon titration by $MgClO_4$ in acetonitrile. Spectral changes around the isosbestic points (257, 273, 309, 330, 349, 424, and 433 nm) are also enlarged. The seven sharp isosbestic points were observed at $[Mg^{2+}] < 7.0 \times 10^{-6}$ M. The isosbestic points except for those at 257 and 433 nm shifted to shorter wavelength with increasing in $[Mg^{2+}]$. These data manifest the present system is a multi-component system.

Table S1. Molar absorption coefficients (ε_X / 10^4 $M^{-1}cm^{-1}$) of the [**1** – M^{2+}] complexes evaluated by the analysis of the titration curves in Figs. 5 and S3.

	Mg^{2+}			Ca^{2+}			Ba^{2+}			Zn^{2+}		
	270 nm	273 nm	470 nm	261 nm	270 nm	450 nm	251 nm	261 nm	450 nm	263 nm	284 nm	465 nm
ε_L	3.97	2.74	0.0123	6.14	3.97	0.181	5.79	6.64	0.181	7.00	2.40	0.0187
ε_{ML}	3.29	3.31	0.751	4.65	4.23	1.25	7.40	5.13	0.997	4.59	4.65	1.78
ε_{ML2}	5.72	5.76	1.81	7.68	6.65	2.23	13.4	11.3	1.26	6.90	6.79	1.80
ε_{ML3}	8.16	8.24	3.28	14.0	11.5	2.93	16.8	18.9	1.8	10.8	10.9	5.17