Supplementary Information (SI) for Soft Matter.
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Supporting Information

Determination of divalent metal ions regulated proton concentration and polarity at the interface of anionic phospholipid membrane

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Table S1 Different bivalent metal ion concentration dependent zeta potential (ZP) for various lipid LUV system. [a]

M^{2+}	$[M^{2+}]$ (mM)	ZP (mV)		
		DMPG	DOPG	POPG
	Absence	–61.0	–58.7	–54.4
Ca^{2+}	0.1	–60.5	–57.0	–53.6
	0.2	–58.0	–55.8	–52.0
	0.3	–56.5	–53.5	–50.2
Mg^{2+}	0.1	–59.0	–57.1	–53.9
	0.2	–58.6	–55.8	–52.7
	0.3	–56.9	–53.9	–51.3
Zn^{2+}	0.1	–59.6	–57.3	–53.7
	0.3	–58.3	–56.2	–52.8
	0.5	–56.3	–54.5	–51.6

[a] Lipid concentration was 1 mM

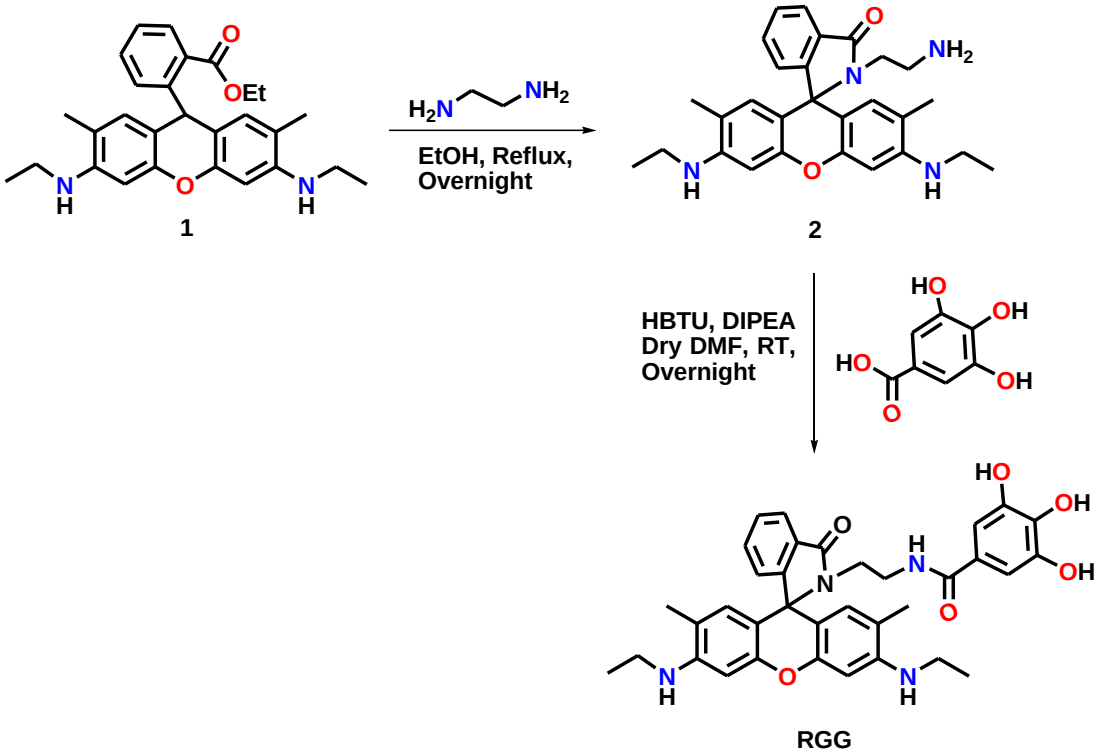

Fig. S1. Synthetic procedure of compound RGG.

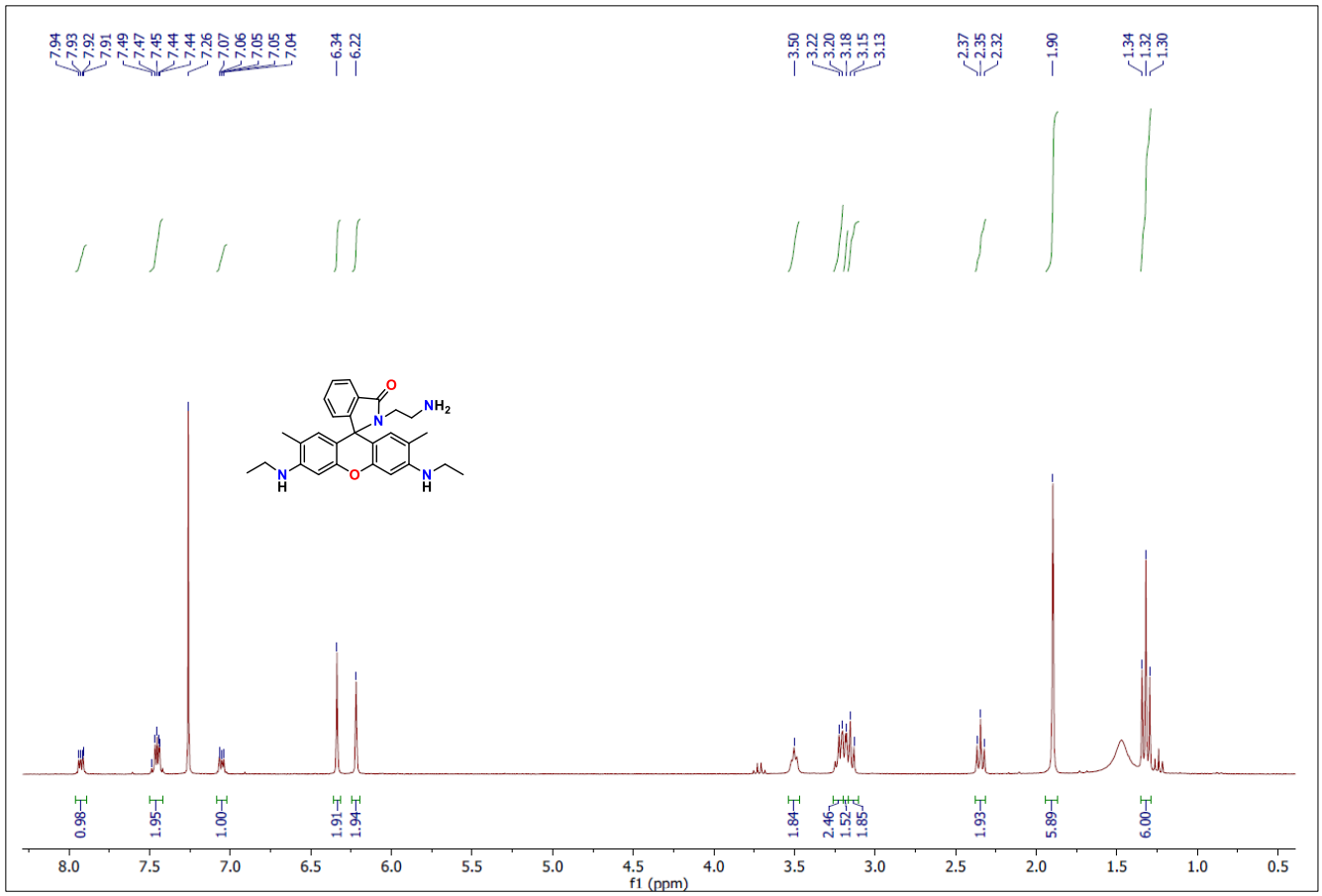

Fig. S2. ^{1}H NMR spectra of compound **2** in $CDCl_3$ as a solvent.

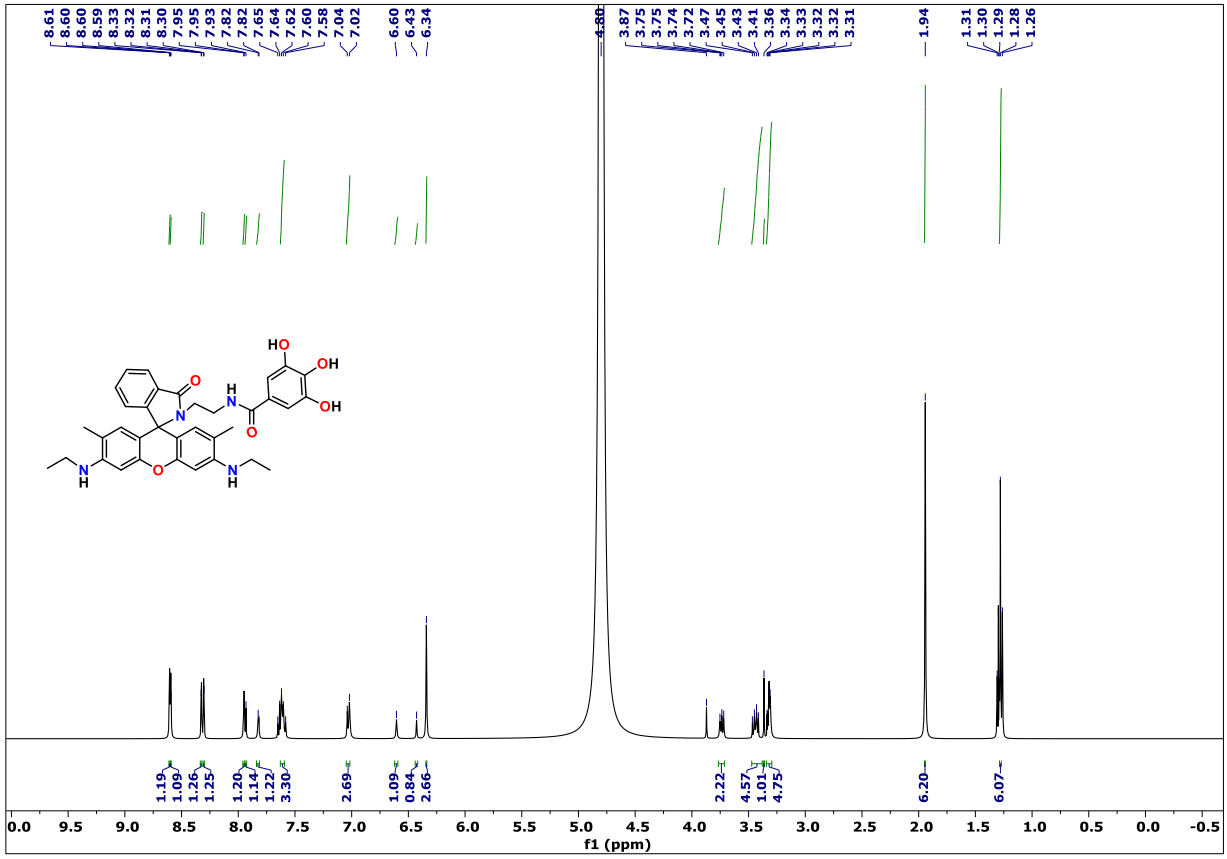

Fig. S3. ^{1}H NMR spectra of compound RGG in D_2O as a solvent.

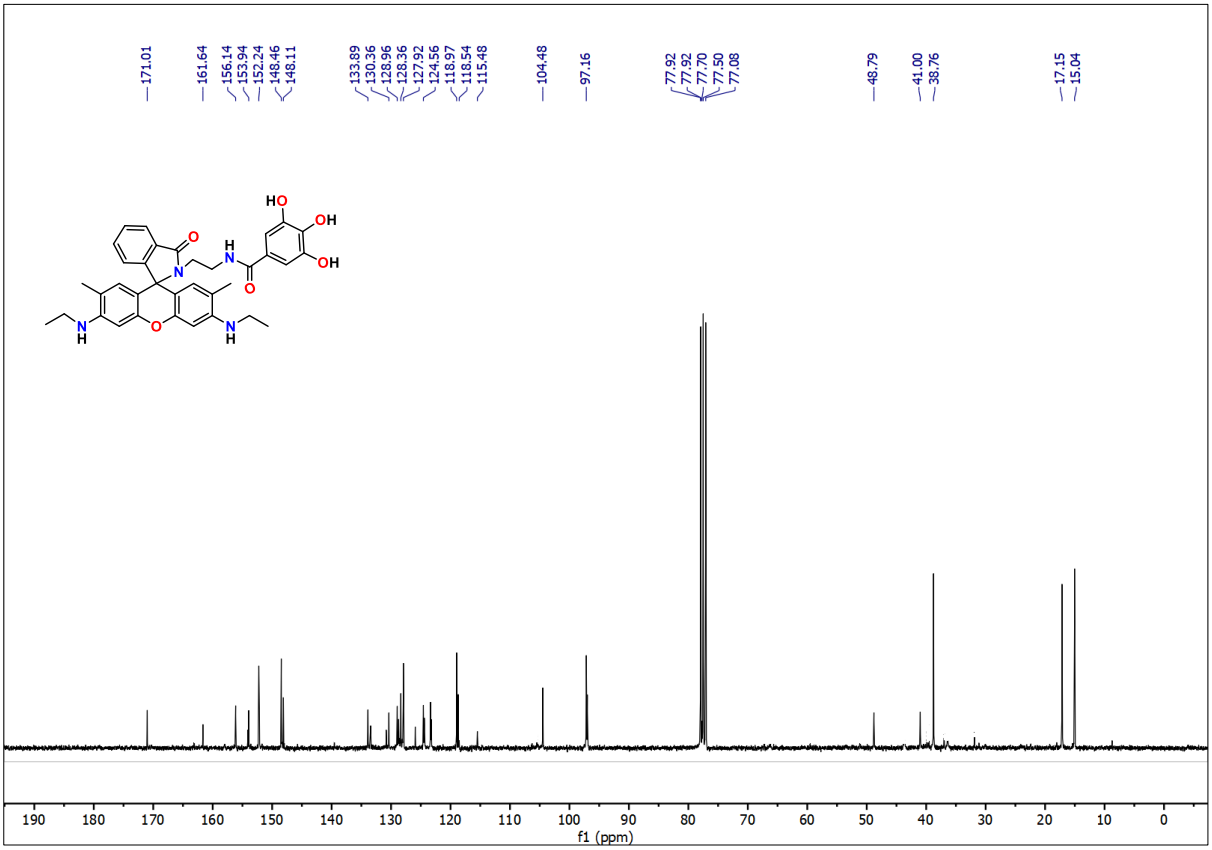

Fig. S4. ^{13}C NMR spectra of compound RGG in $CDCl_3$ as a solvent.

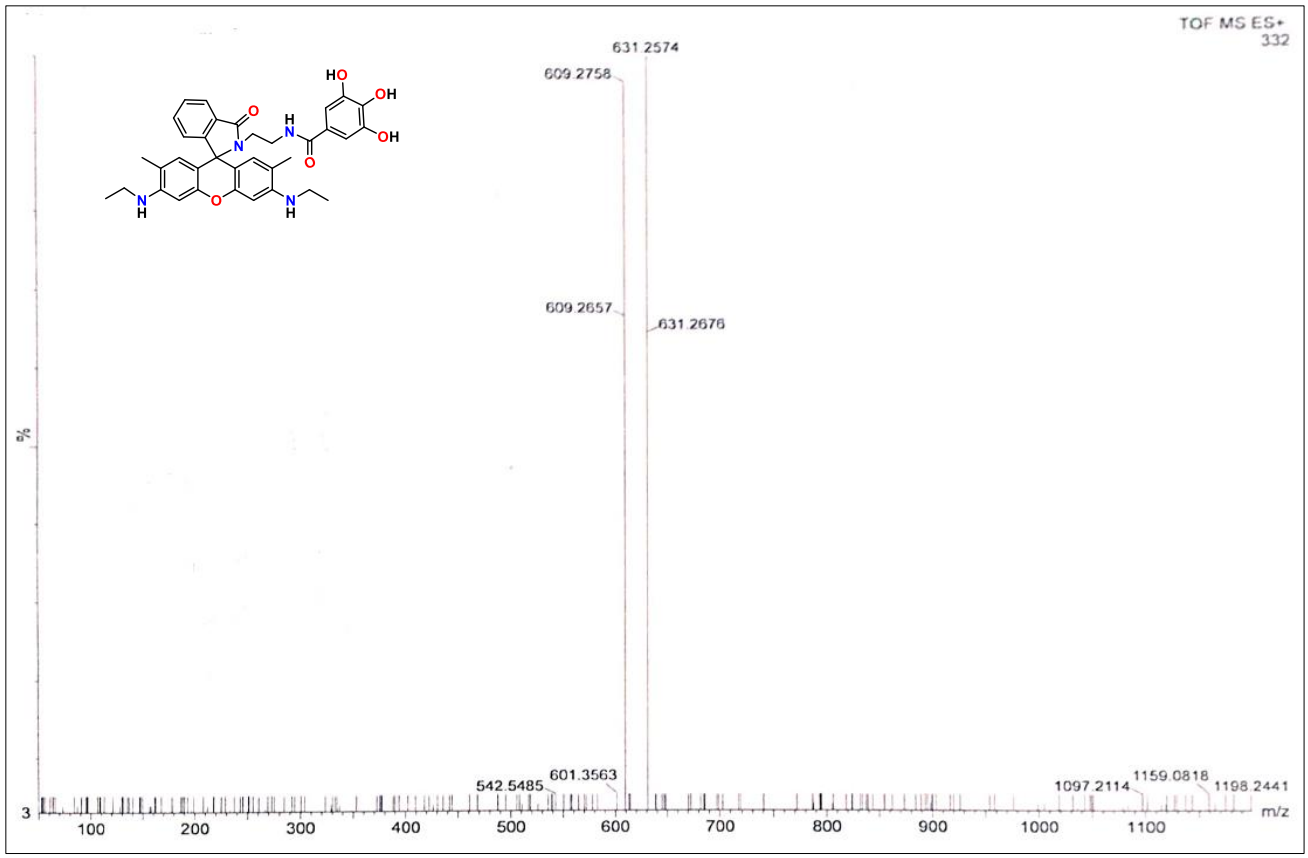

Fig. S5. HR-MS spectrum of compound RGG.

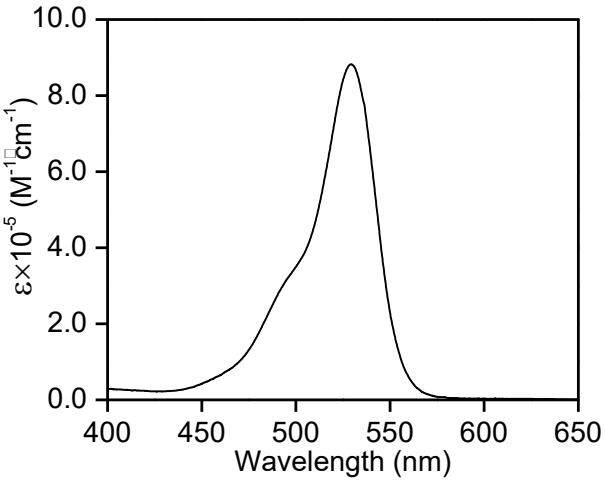

Fig. S6. UV-Vis absorption spectrum of RGG (2 μM) in 2 mM Britton–Robinson buffer, at pH 2.5. The spectrum was recorded 1 hours after addition of RGG.

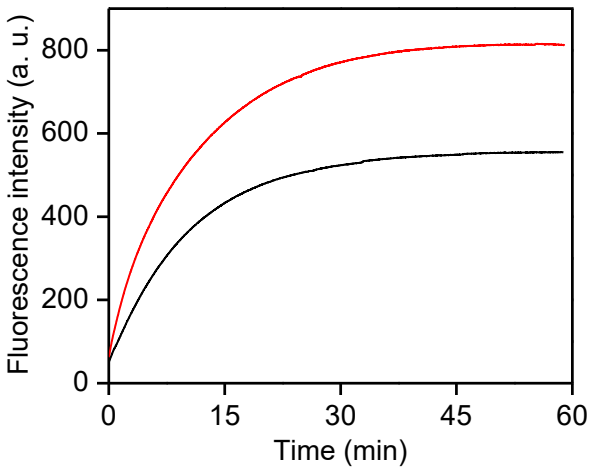

Fig. S7. Changes of fluorescence intensities of RGG at 555 nm in absence (black) and presence (red) of DMPG (1 mM) LUV were plotted against of exposure time of RGG in 2 mM Britton–Robinson buffer, pH 2.5 (black) or HEPES, pH 5.5 at 25 °C. Excitation and emission wavelengths were 530 and 560 nm.

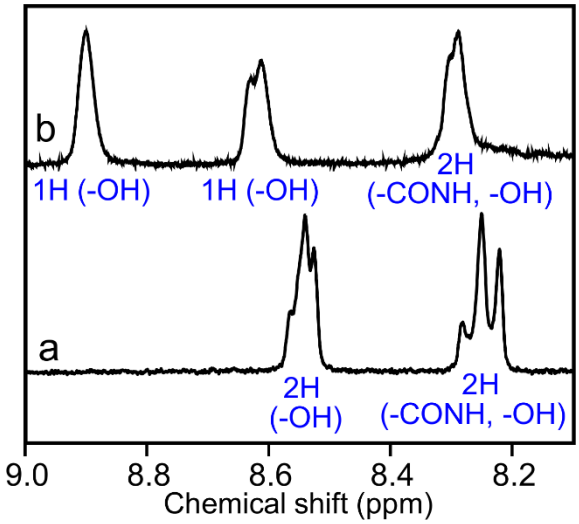

Fig. S8. ^{1}H NMR spectra of RGG (1.0 mM) in the downfield region in (a) D_2O and (b) 6:4 DMSO-d_6 and D_2O medium.

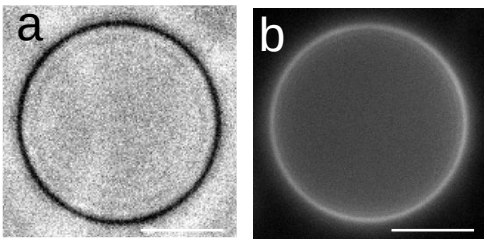

Fig. S9. (a) Phase contrast and (b) fluorescence microscopic observation of DOPG/DOPC (2:1) GUVs (total lipid, 0.5 mM) in 1 mM HEPES buffer, pH 7.0, containing 200 mM sucrose at 25°C. Images were captured after 2 hours of RGG (0.5 μM) addition in the solution. White bars represent 5 μm.

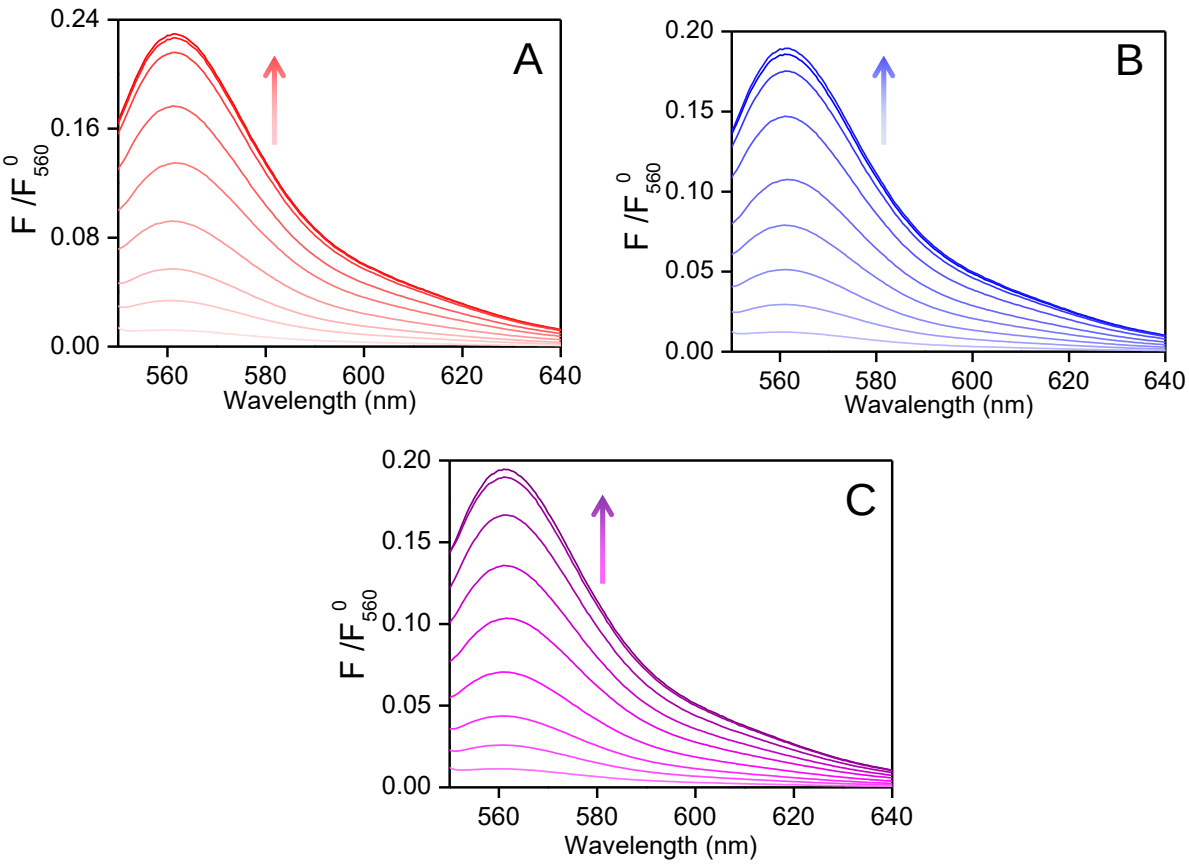

Fig. S10. LUV-concentration dependence (lipid, 0–1.0 mM) of normalized fluorescence spectra of RGG (1 μM) in the presence of LUVs: (A) DMPG, (B) DOPG and (C) POPG LUVs in 2 mM HEPES, pH 7.0 at 25°C. The increases in intensities by increasing the LUV concentrations are indicated in arrows. *F* represents the fluorescence intensity at pH 7.0, and F^0_{560} represents *F* at pH 5.5. Excitation wavelength was 530 nm.

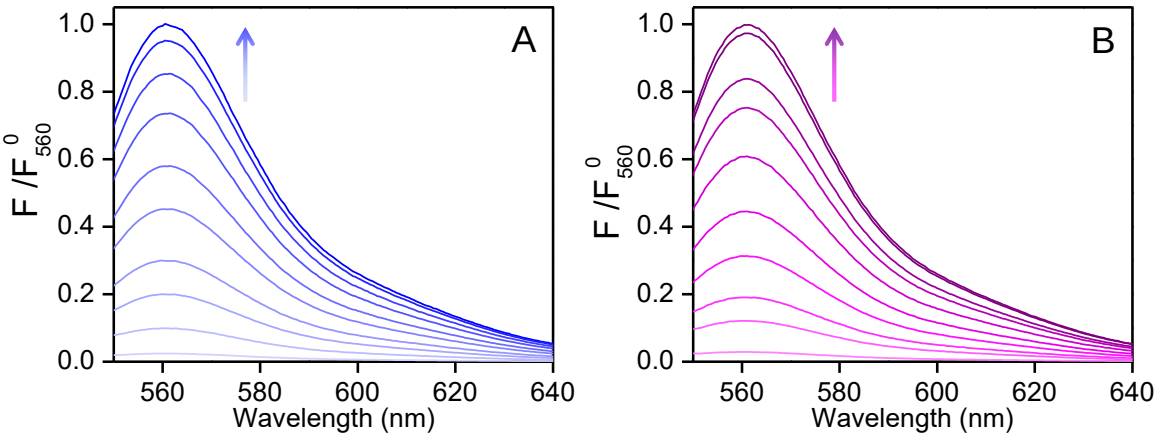

Fig. S11. Normalized fluorescence spectra of RGG (1 μM) in the presence of binding saturated concentration of (A) DOPG and (B) POPG LUV (1 mM) at various pH: 7.50, 7.25, 7.00, 6.80, 6.60, 6.40, 6.20, 6.00, 5.75, 5.50. *F* represents the fluorescence intensity, and F^0_{560} represents *F* at pH 5.5. The intensity changes by decreasing pH are shown in arrows. Excitation wavelength was 530 nm.

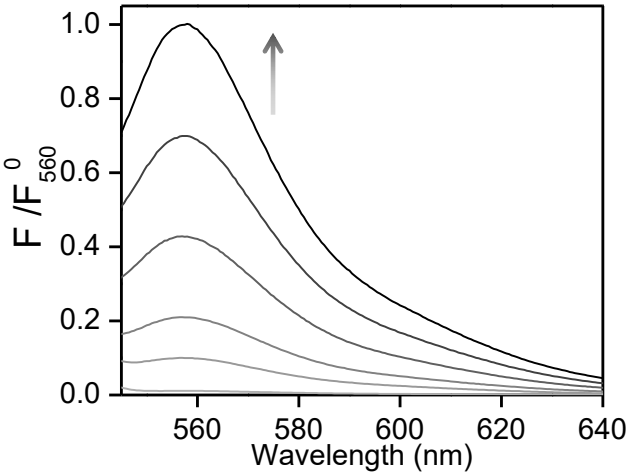

Fig. S12. Normalized fluorescence spectra of RGG (1 μM) in in 2 mM Britton–Robinson buffer containing 30% (v/v) ethanol at various pH: 4.50, 4.00, 3.80, 3.40, 3.00 and 2.25. F represents the fluorescence intensity, and F^0_{560} represents F at pH 5.5. The intensity changes by decreasing pH are shown in arrows. Excitation wavelength was 530 nm.

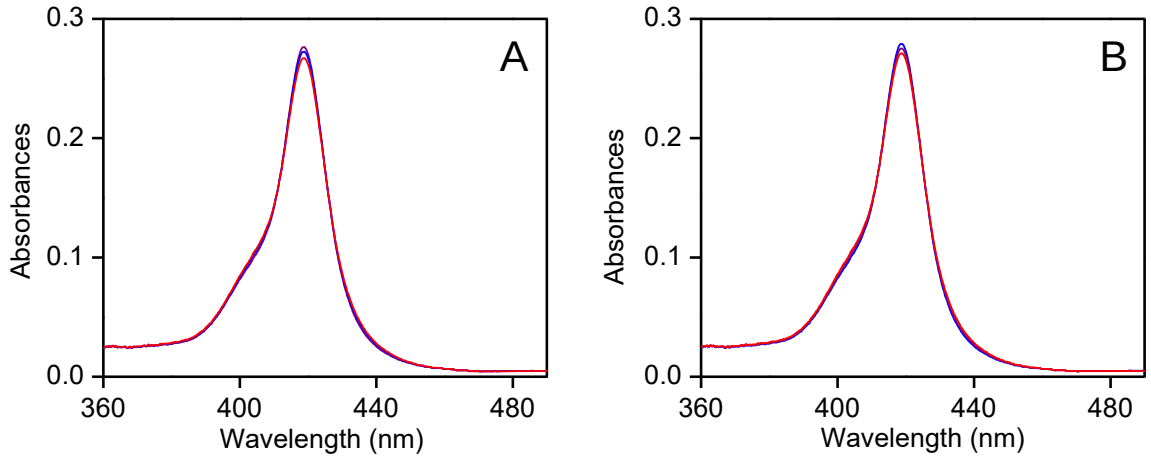

Fig. S13. UV-Vis absorption spectra of GPP (2.5 μM)) in the presence of binding saturated concentration of DMPG (red), DOPG (blue) and POPG (purple) LUV (1 mM) in 2 mM HEPES buffer at different pH values: (A) 7.0 and (B) 6.0 at 25 °C.

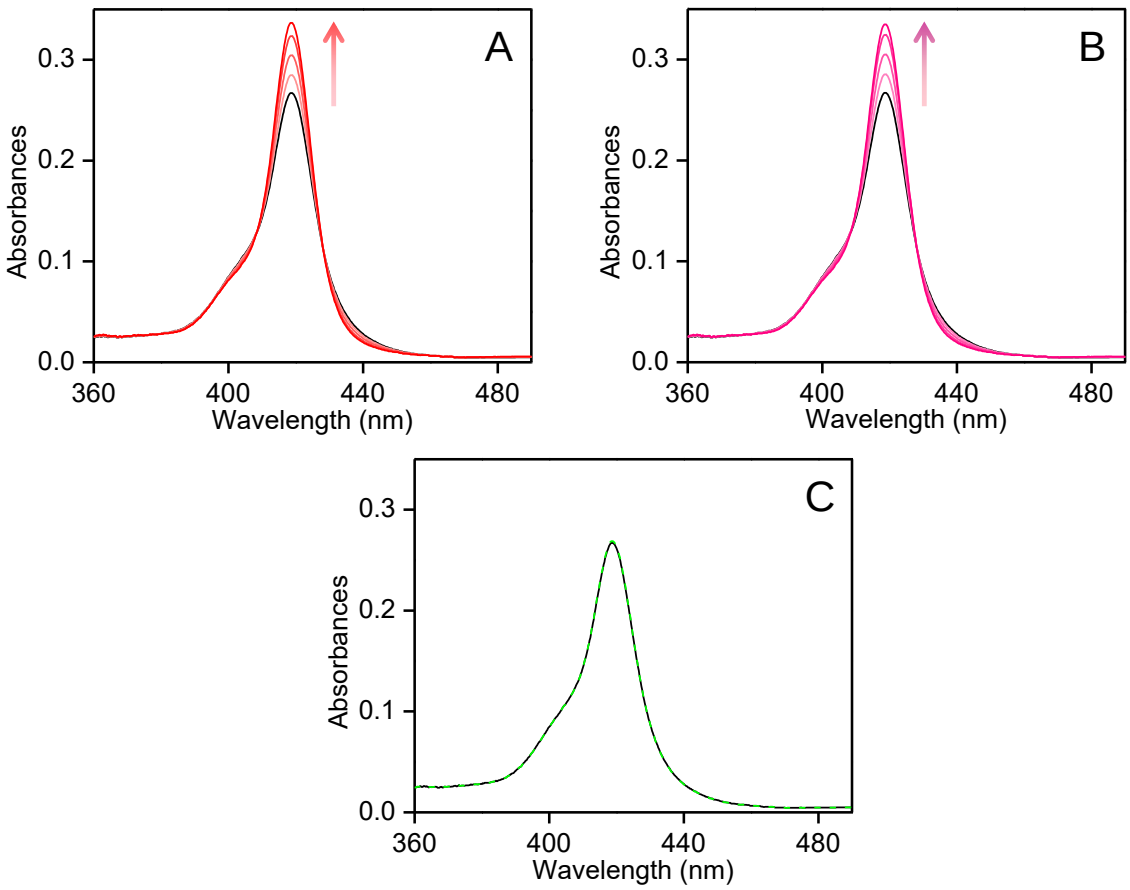

Fig. S14. (A) Ca^{2+}, (B) Mg^{2+} and (C) Na^{+} ion concentration (0.03–0.5 mM for Ca^{2+}/Mg^{2+}; 1.0 mM for Na^{+}) dependent UV-Vis absorption spectra of GPP (2.5 μM)) in the presence of binding saturated concentration of DMPG LUV (1 mM) in 2 mM HEPES buffer, pH values at 25 °C. (A–C) The spectra in the absence of metal ions are depicted by black. (A,B) The intensity changes by increasing metal ion concentration are shown in arrows.

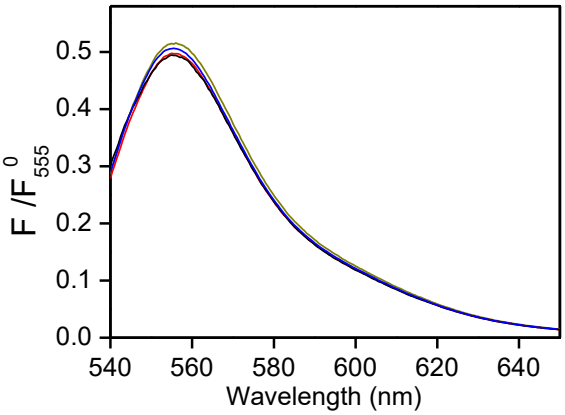

Fig. S15. Normalized fluorescence spectra of RGG (1 μM) in the presence of different bivalent metal ions (0.5 mM) in 2 mM Britton–Robinson buffer, pH 3.7: red, Ca^{2+}; blue, Mg^{2+} and orange, Zn^{2+}. The spectrum in the absence of metal ions is shown by black. *F* represents the fluorescence intensity, and F^0_{555} represents *F* at pH 2.4. Excitation wavelength was 530 nm.

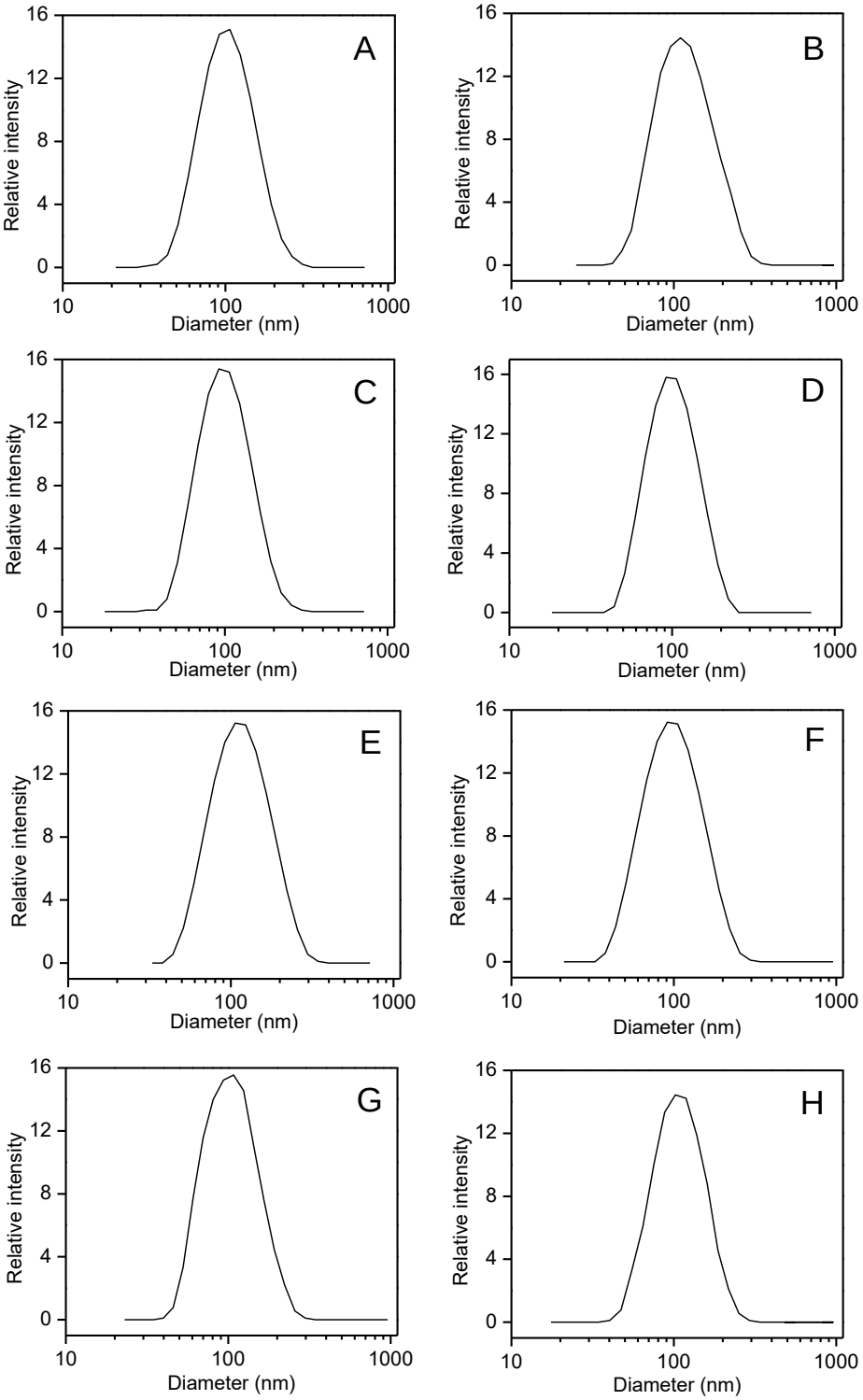

Fig. S16. DLS measurement showing particle size distribution profile of DOPG LUV (1 mM) in the (A,B) absence and (C–H) presence of various mono-valent (1 mM) and bi-valent metal ions (0.3 mM) at pH (A, C–E, H) 7.5 and (B, F, G) 6.0: (C,F) Ca^{2+}, (D,G) Mg^{2+}, (E) Zn^{2+} and (H) Na^{+}. Each of these spectra is an average of 48 scan.

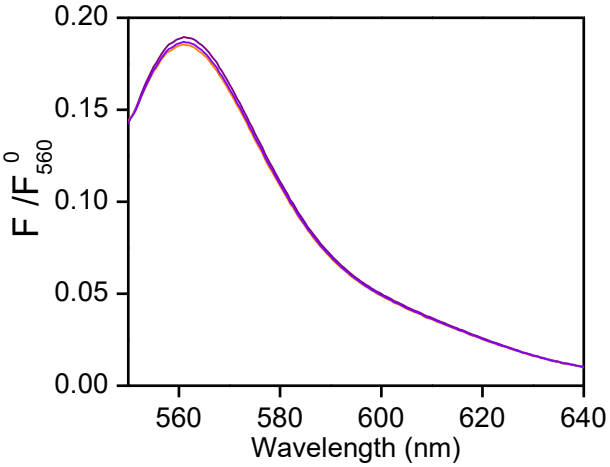

Fig. S17. Normalized fluorescence spectra of RGG (1 μM) in the presence of binding saturated concentration of POPG LUV (1 mM) containing 1.0 mM NaCl (orange) or KCl (violet) in 2 HEPES, pH 7.0. The spectrum in the absence of salts is shown by purple. *F* represents the fluorescence intensity, and F^0_{560} represents *F* at pH 5.5. Excitation wavelength was 530 nm.