Towards understanding the design of dual-modal MR/fluorescent probes to sense zinc ions

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Figure S1: ^{1}H NMR spectrum of **1**, $CDCl_3$, 298 K.

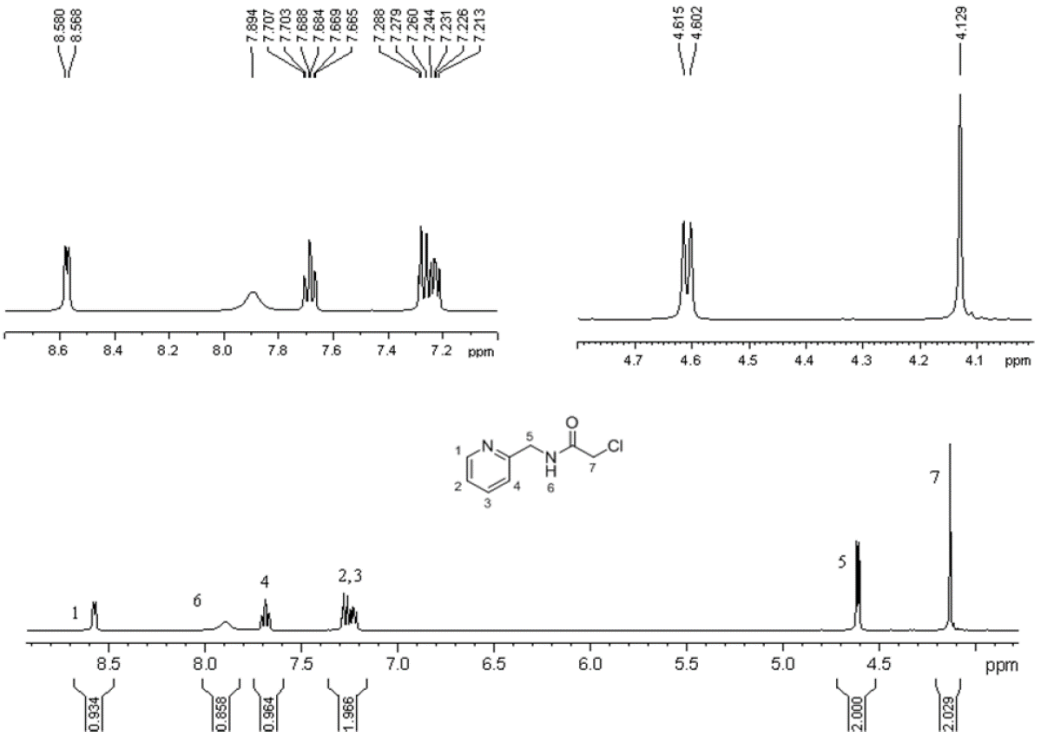

Figure S2: CIMS spectrum of **1**.

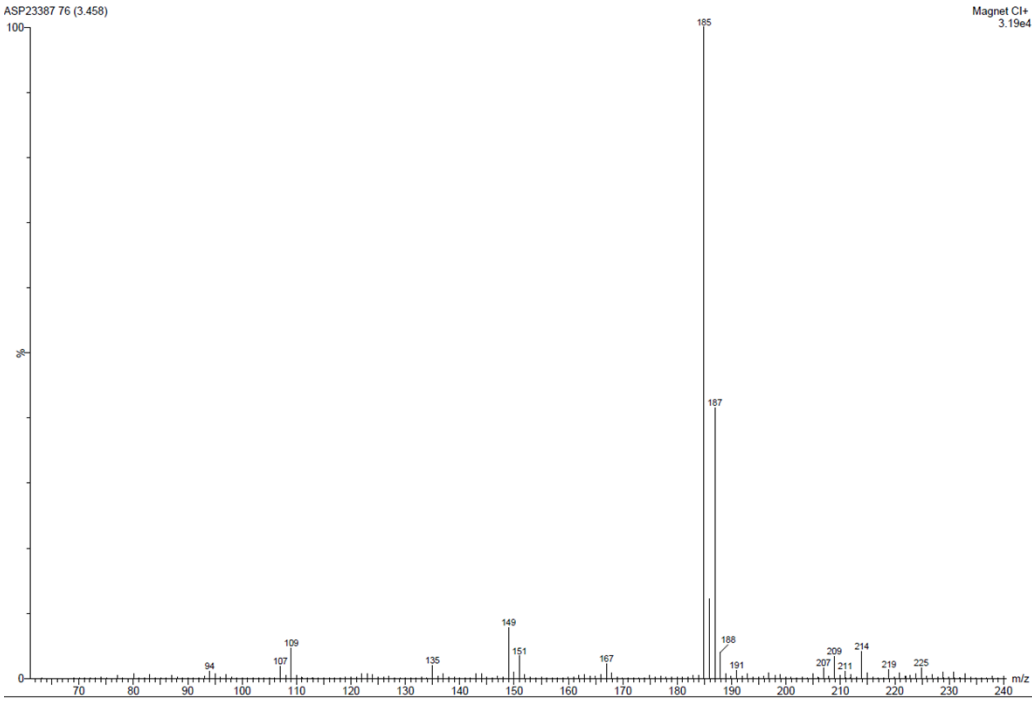

Figure S3: ^{1}H NMR spectrum of **2**, $CDCl_3$, 298 K.

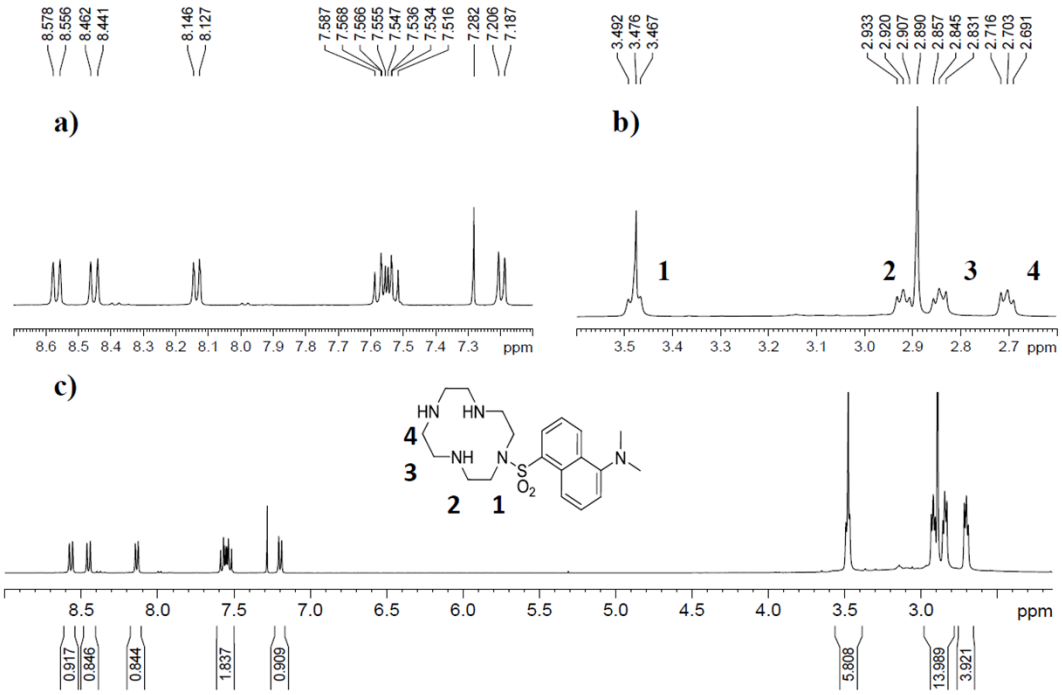

Figure S4: ESMS spectrum of **2**.

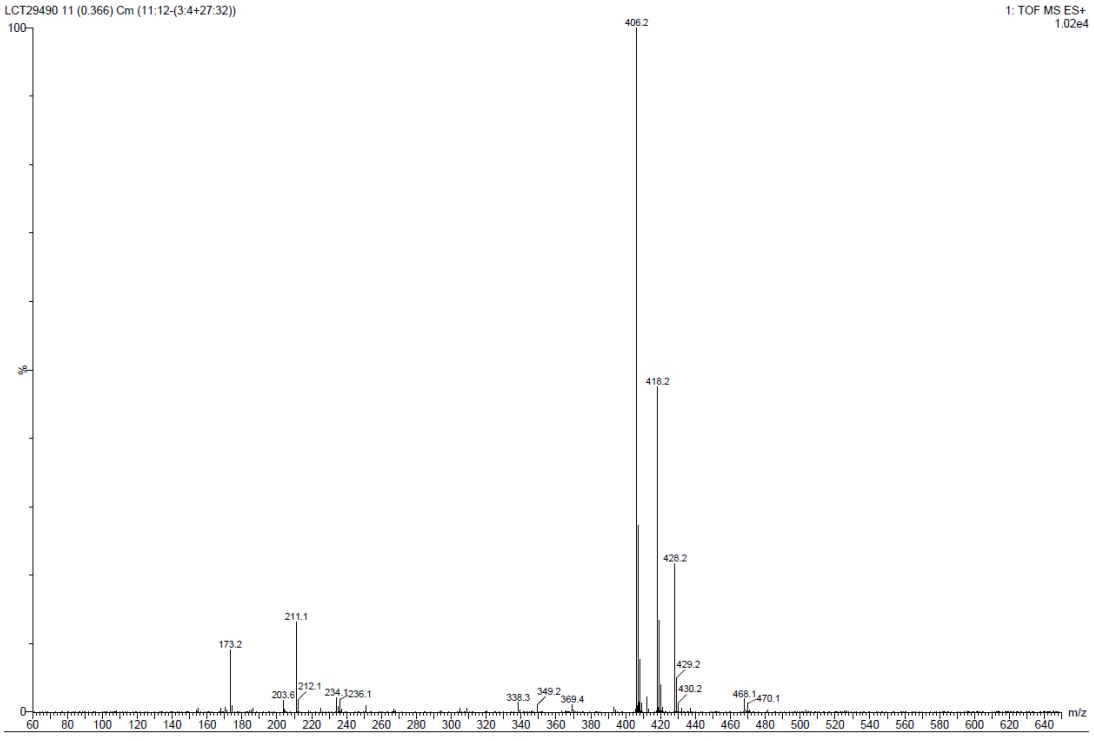

Figure S5: ^{1}H NMR spectrum of **L1**, $CDCl_3$, 298 K.

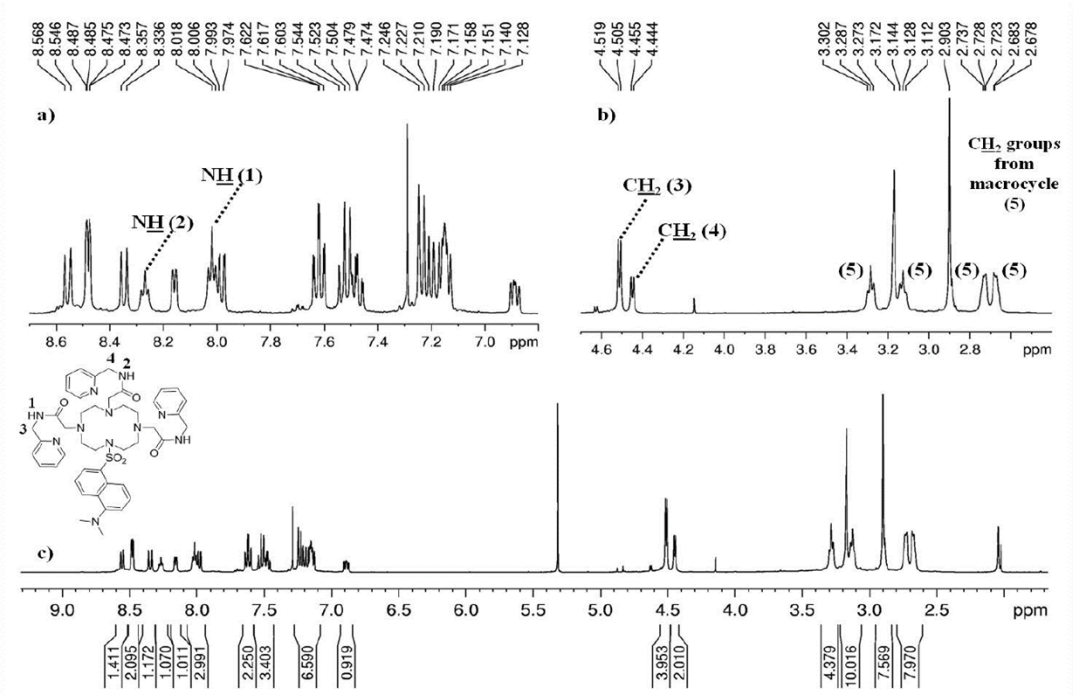

Figure S6: ESMS spectrum of **L1**.

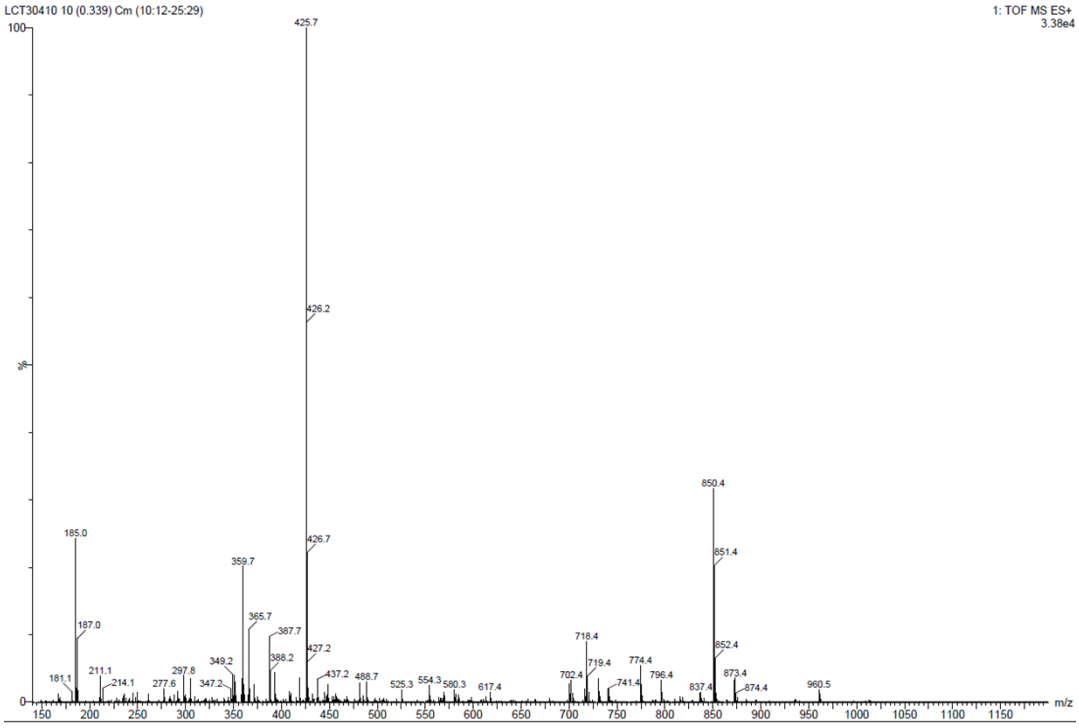

Figure S7. UV/vis. spectra of **GdL^1** (100 μM) in HEPES buffer (0.1 M; pH = 7.4) in the presence of increasing concentrations (0 to 5 eq.) of respective metal ion.

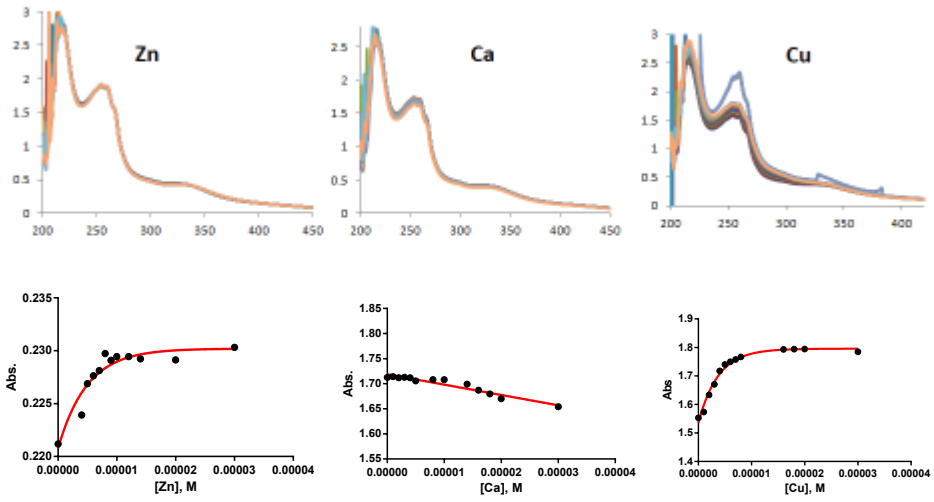

Figure S8. Fluorescence emission spectra of **GdL^1** (1 mM) in 50:50 MeOH:HEPES buffer (0.1 M; pH = 7.4) in the presence of increasing concentrations (0 to 5 eq.) of Ca^{2+}.

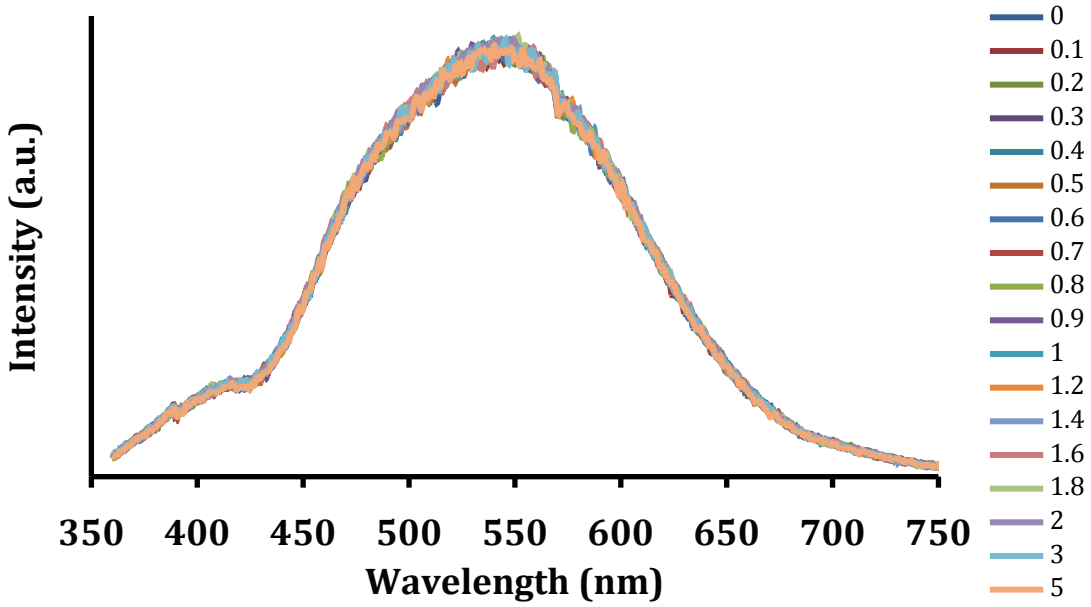

Figure S9: ^{1}H NMR spectrum of **4**, $CDCl_3$, 298 K.

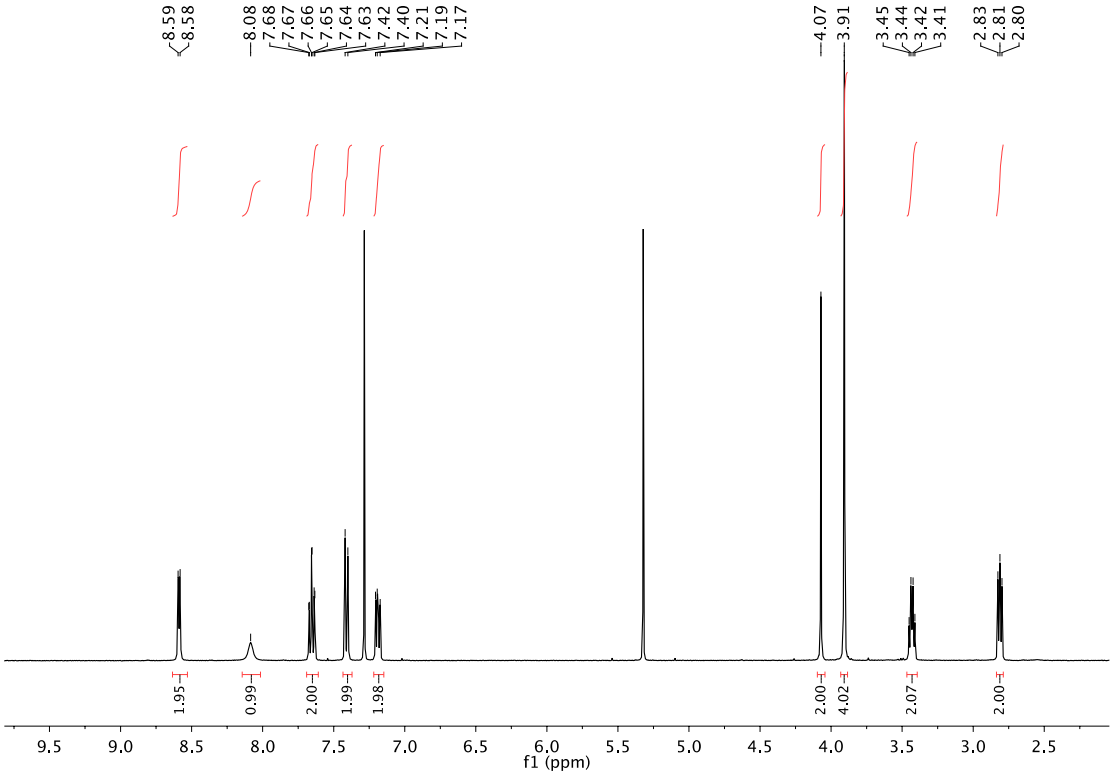

Figure S10: HR ESMS spectrum of **4**.

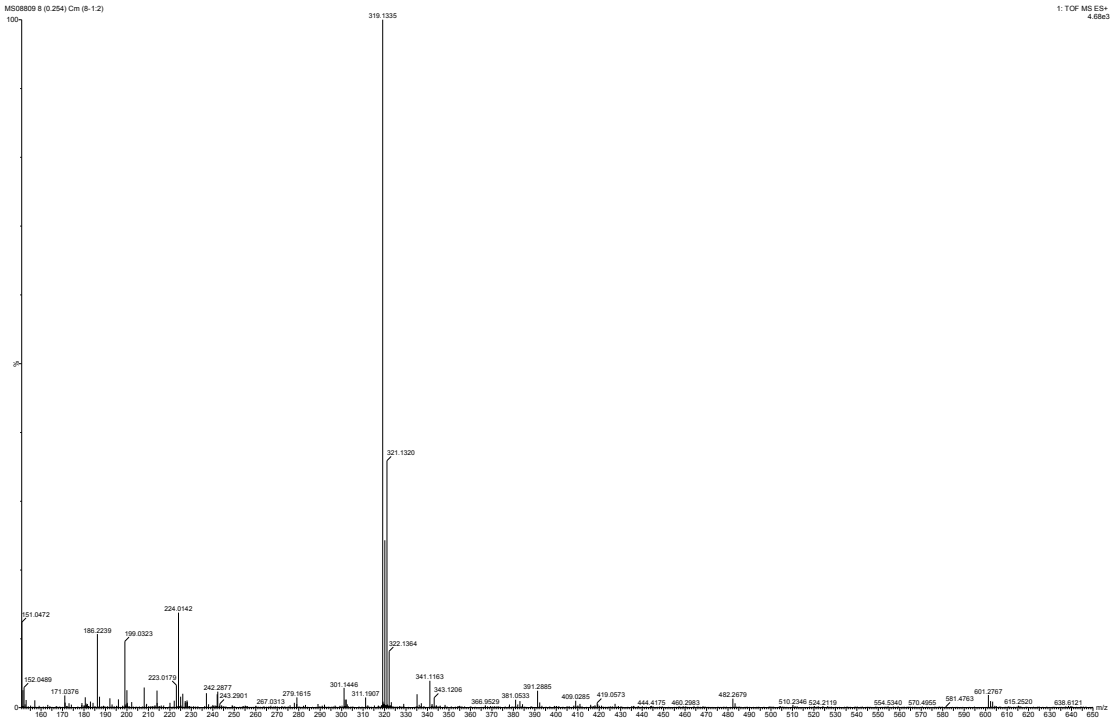

Figure S11: ^{1}H NMR spectrum of **5**, $CDCl_3$, 298 K.

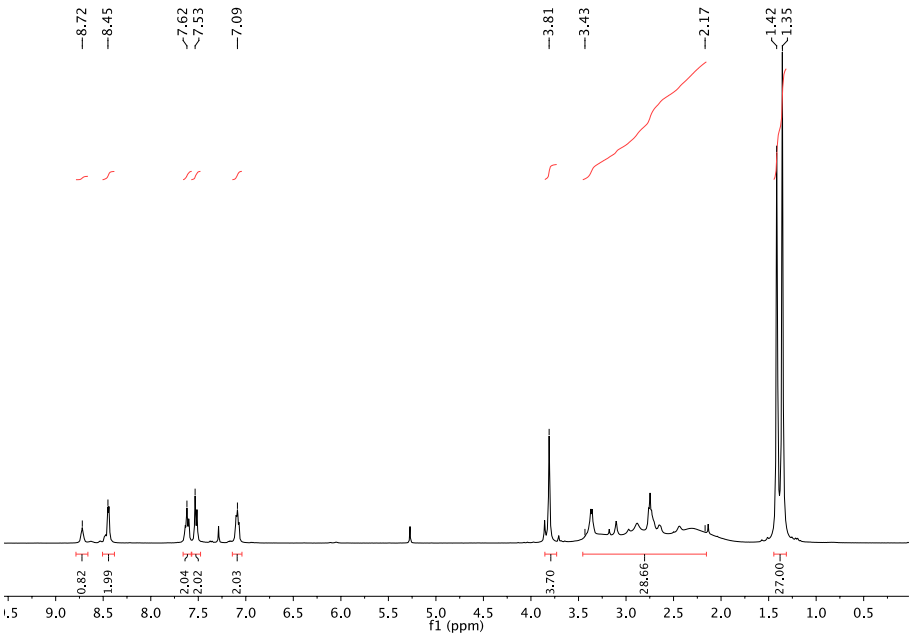

Figure S12: HR ESMS spectrum of **5**.

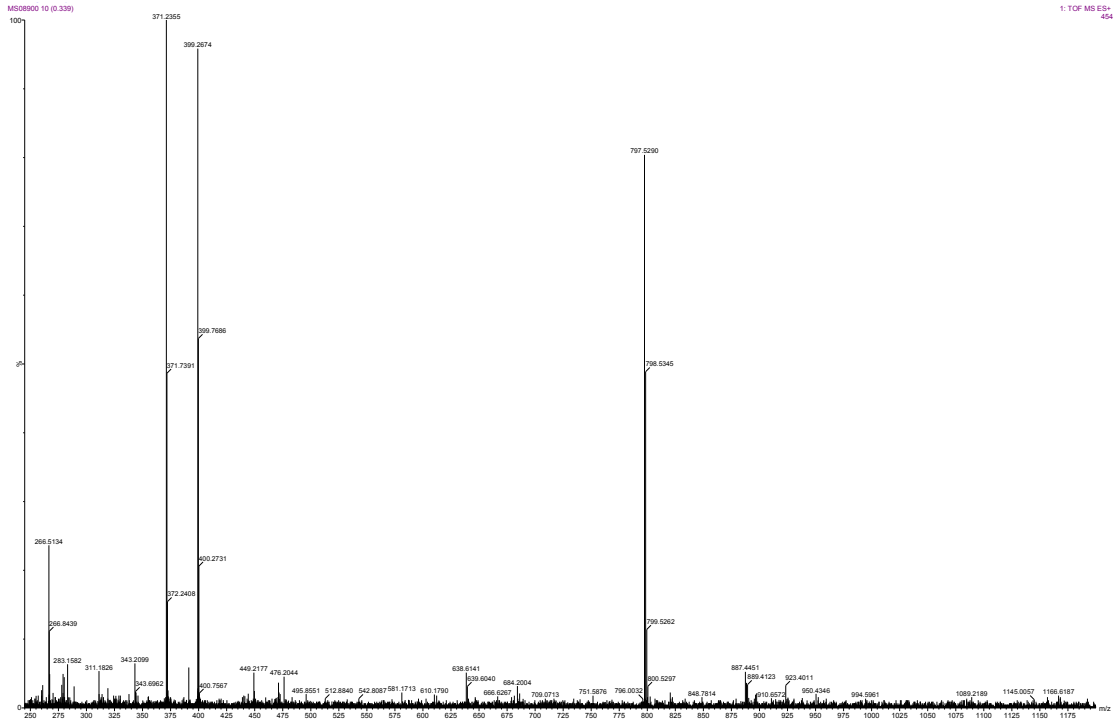

Figure S13: ^{1}H NMR spectrum of **L²**, D_2O, 298 K.

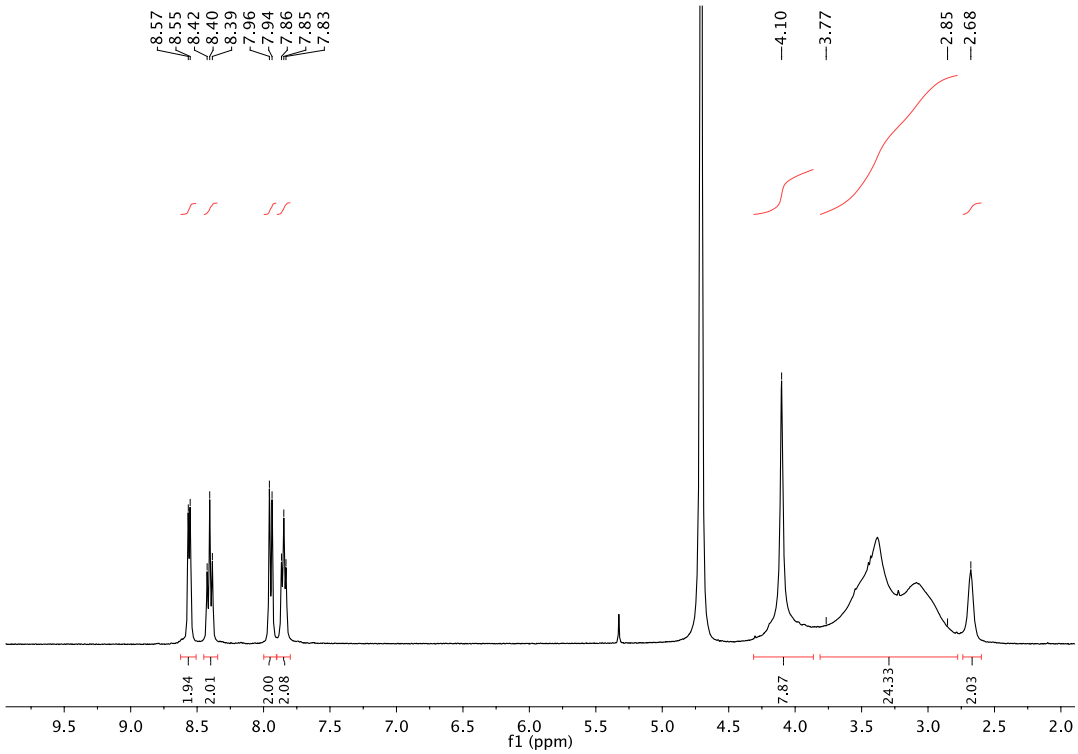

Figure S14: HR ESMS spectrum of **L²**.

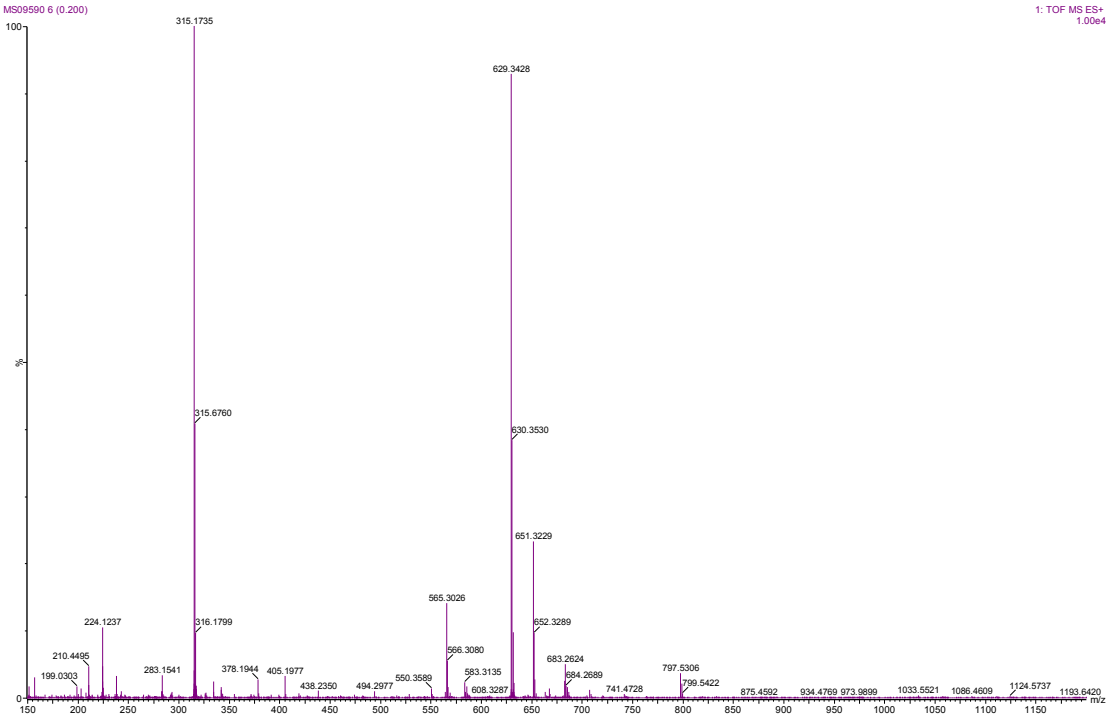

Figure S15: ESI MS spectrum of **GdL²**.

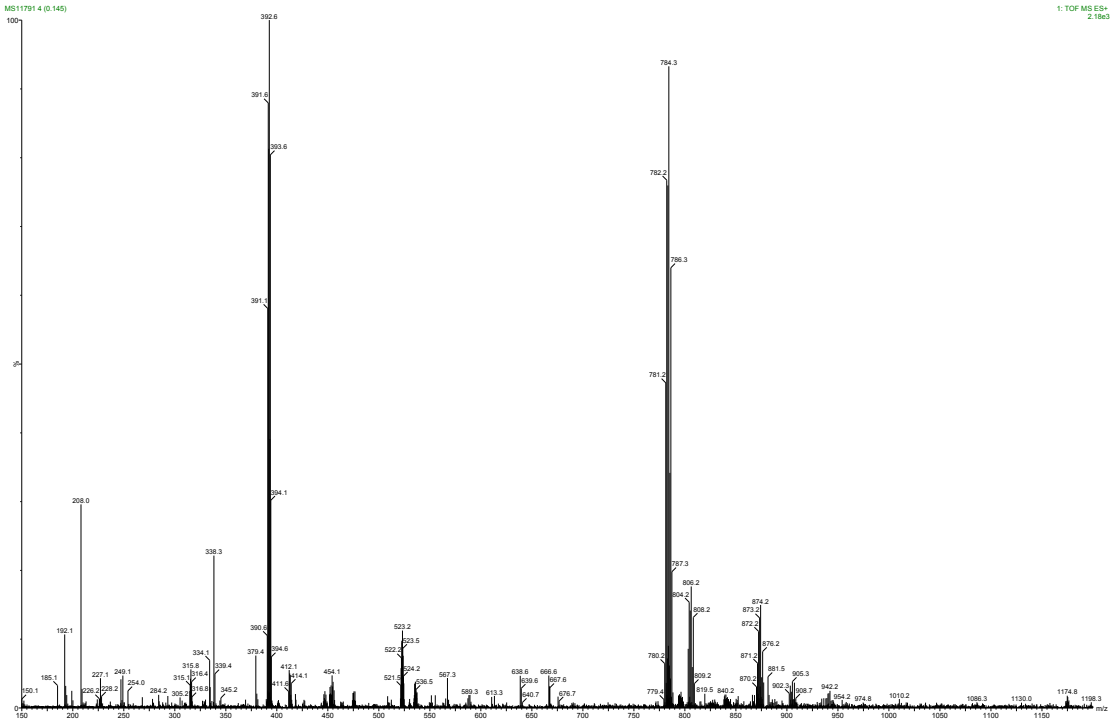

Figure S16: UV/vis. spectra of **GdL²** (100 μM) in HEPES buffer (0.1 M; pH = 7.4) in the presence of increasing concentrations (0 to 5 eq.) of Cu^{2+}.

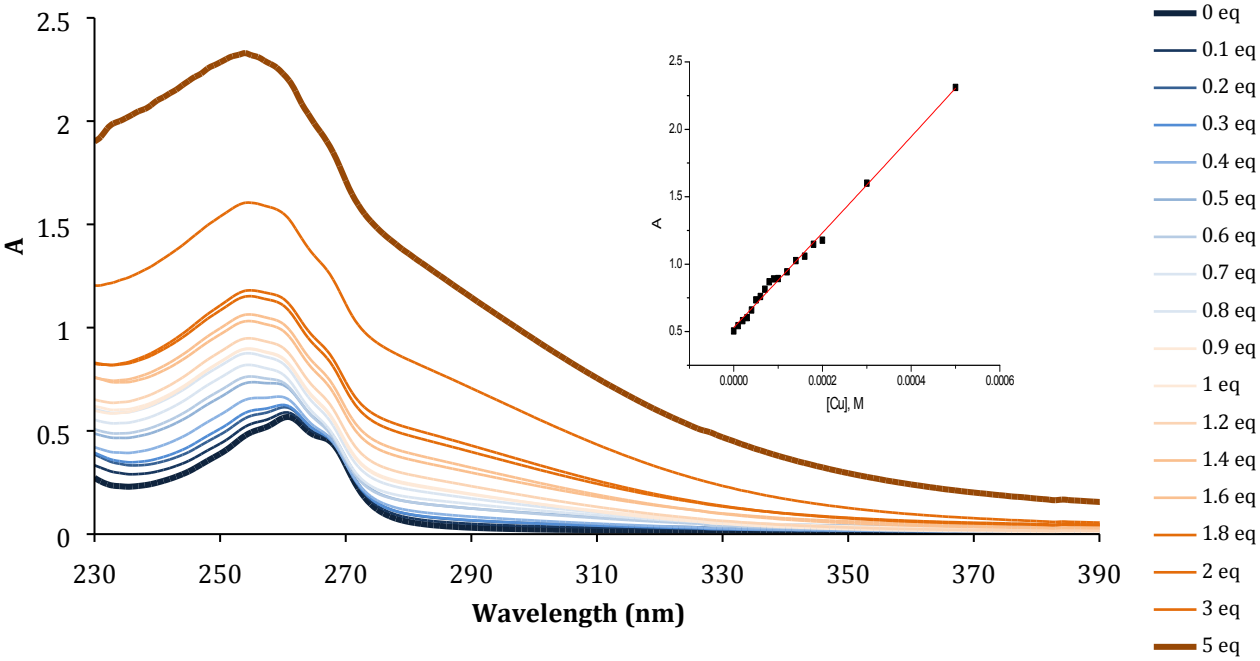

Figure S17. UV/vis. spectra of **GdL²** (100 μM) in HEPES buffer (0.1 M; pH = 7.4) in the presence of increasing concentrations (0 to 5 eq.) of Ca^{2+}.

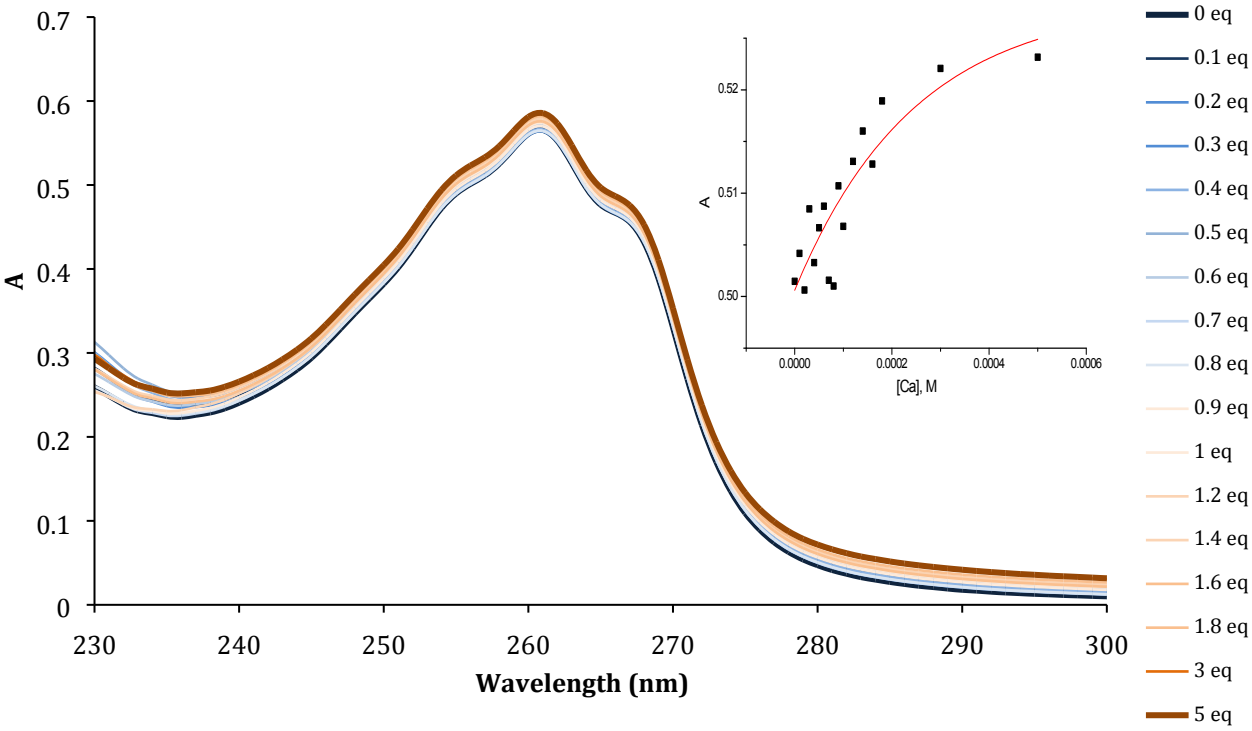

Figure S18. UV/vis. spectra of **GdL²** (100 μM) in HEPES buffer (0.1 M; pH = 7.4) in the presence of increasing concentrations (0 to 5 eq.) of Mg^{2+}.

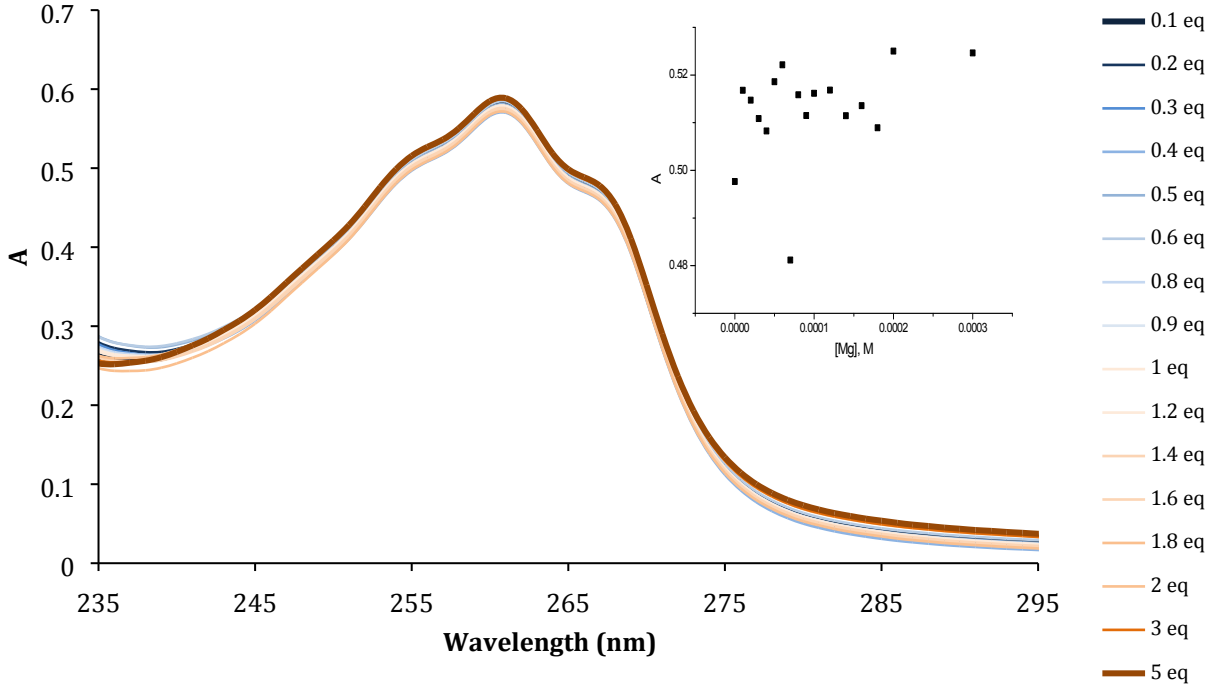

Figure S19: ^{1}H NMR spectrum of **6**, $CDCl_3$, 298 K.

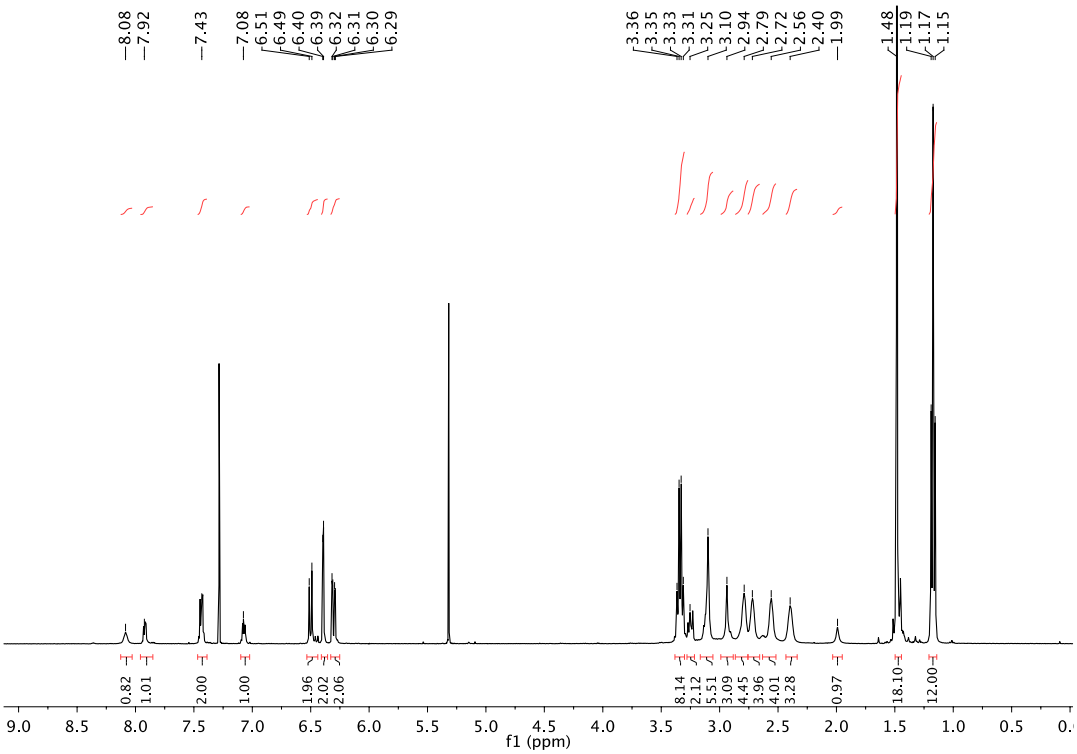

Figure S20: HR ESMS spectrum of **6**.

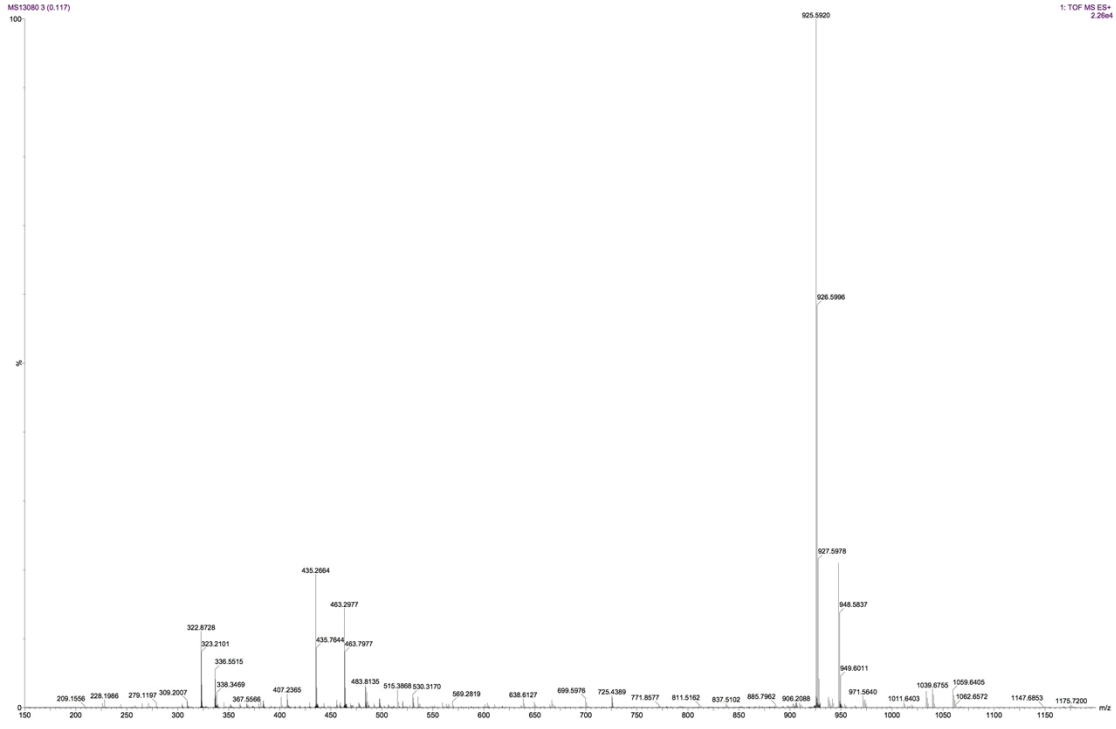

Figure S21: ^{1}H NMR spectrum of **7**, $CDCl_3$, 298 K.

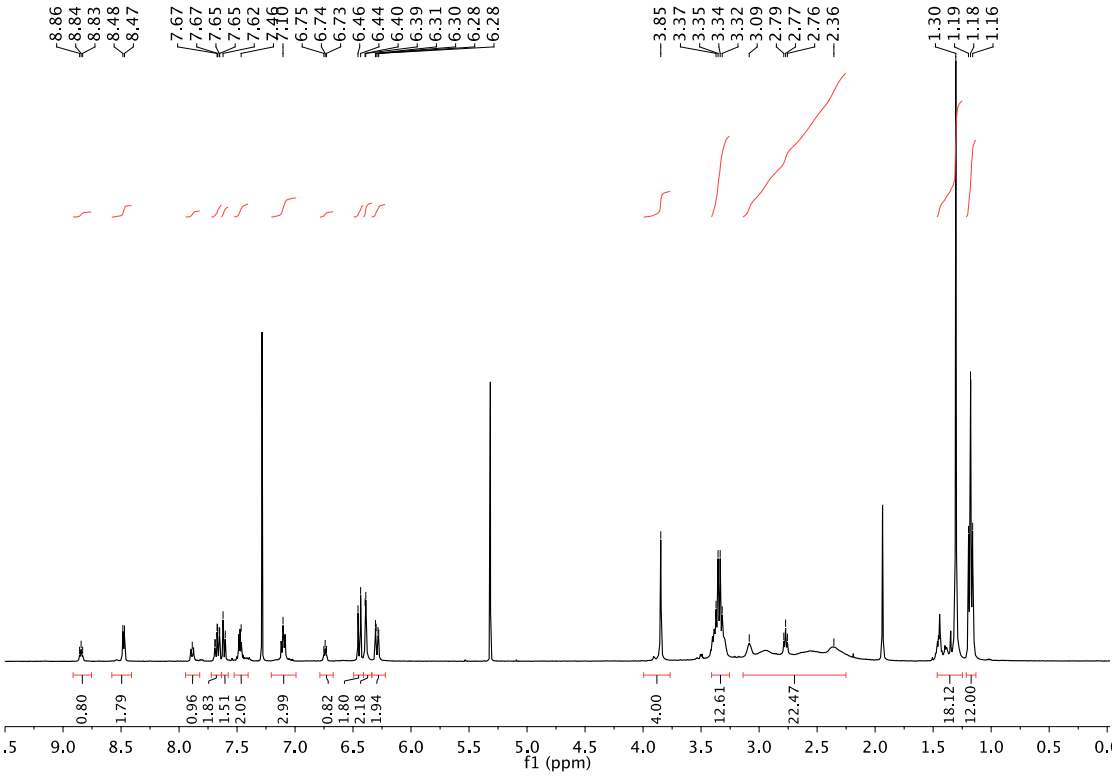

Figure S22: HR ESMS spectrum of **7**.

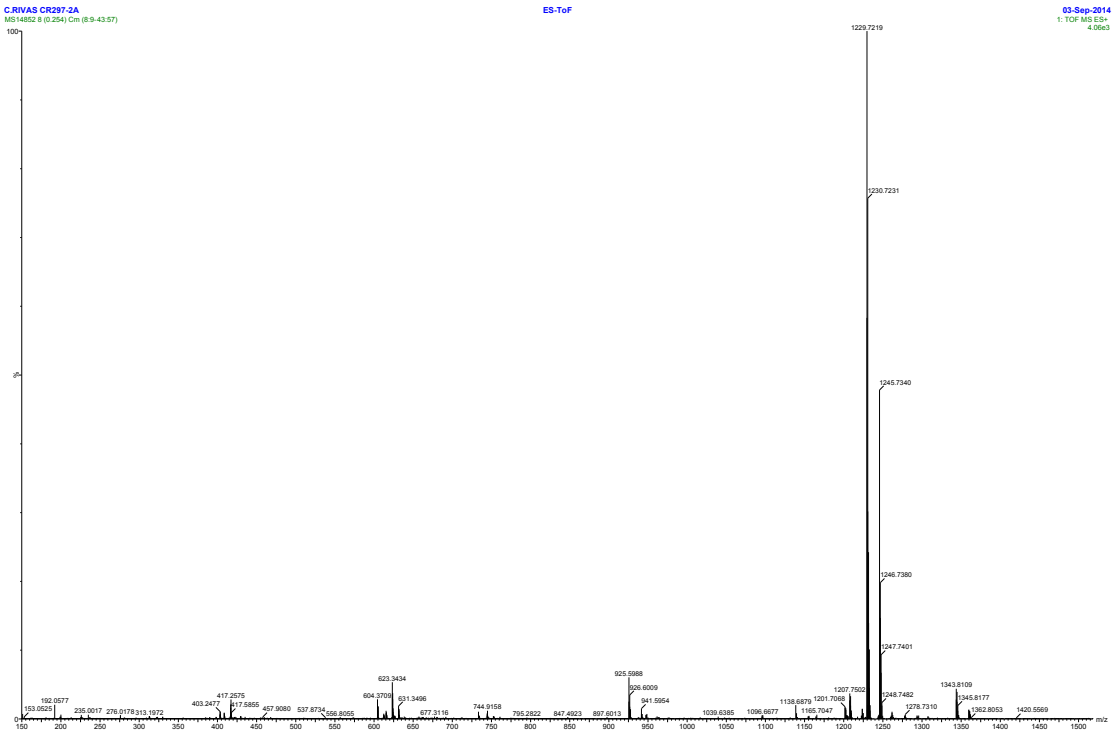

Figure S23: ^{1}H NMR spectrum of **L^{3}**, $CDCl_3$, 298 K.

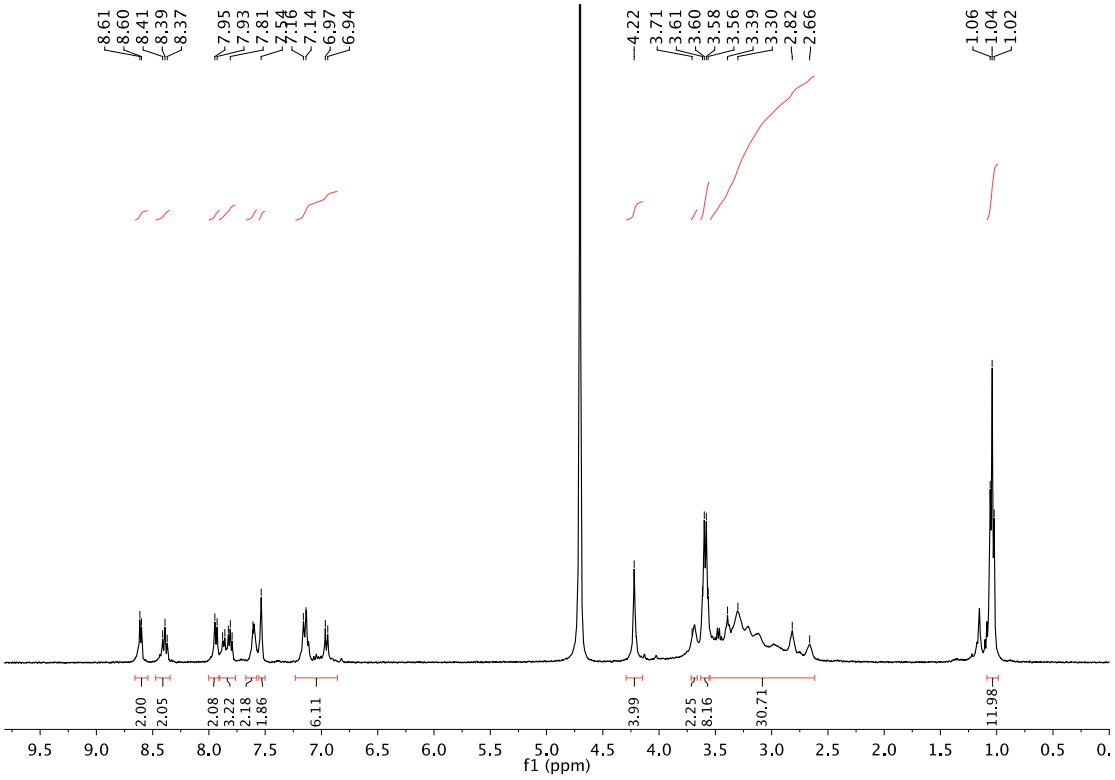

Figure S24: HR ESMS spectrum of **L^{3}**.

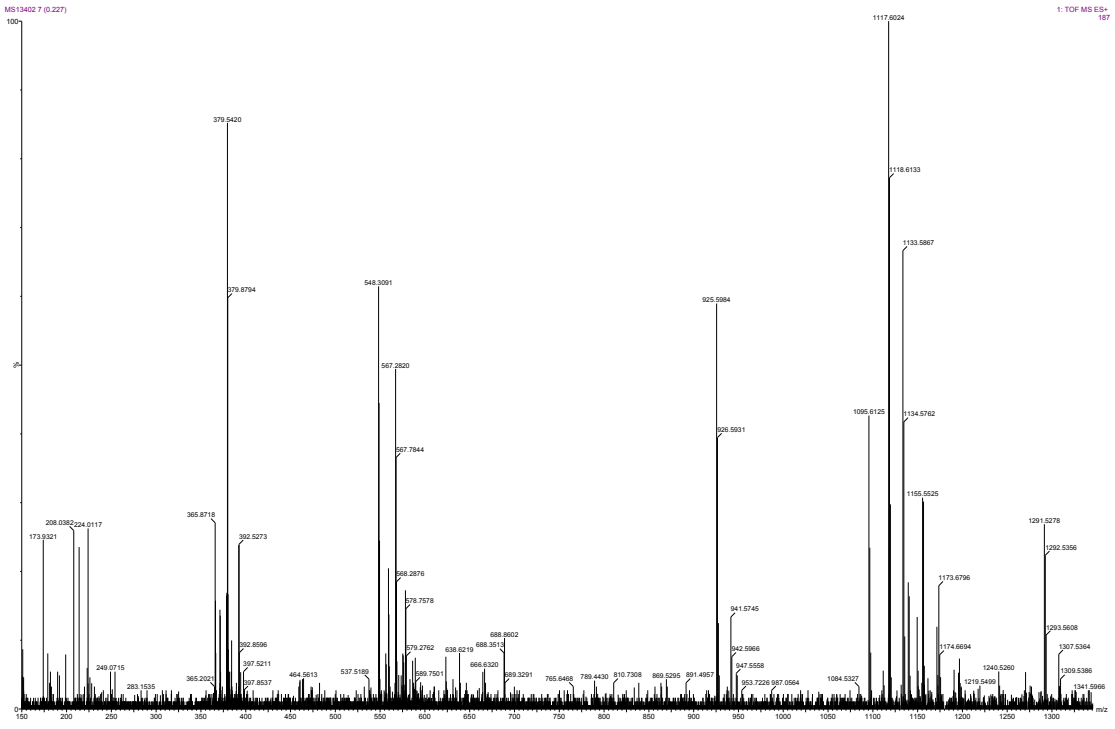

Figure S25: HR ESMS spectrum of **GdL^3**.

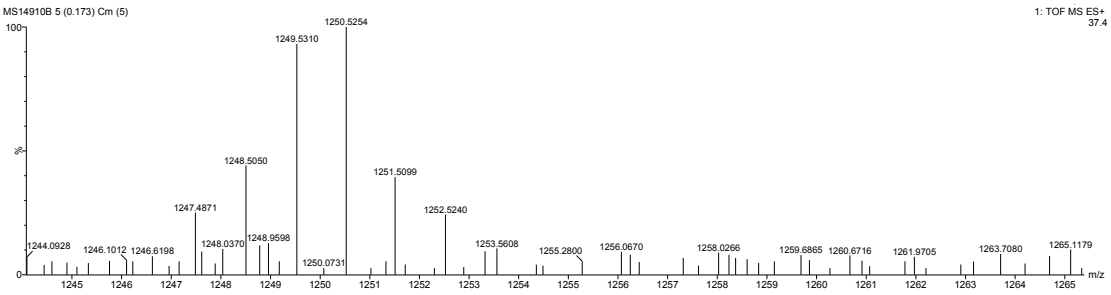

Figure S26: UV-vis spectrum of **GdL^3** (100 μM) in 50:50 MeOH:HEPES buffer (0.1 M; pH = 7.4).

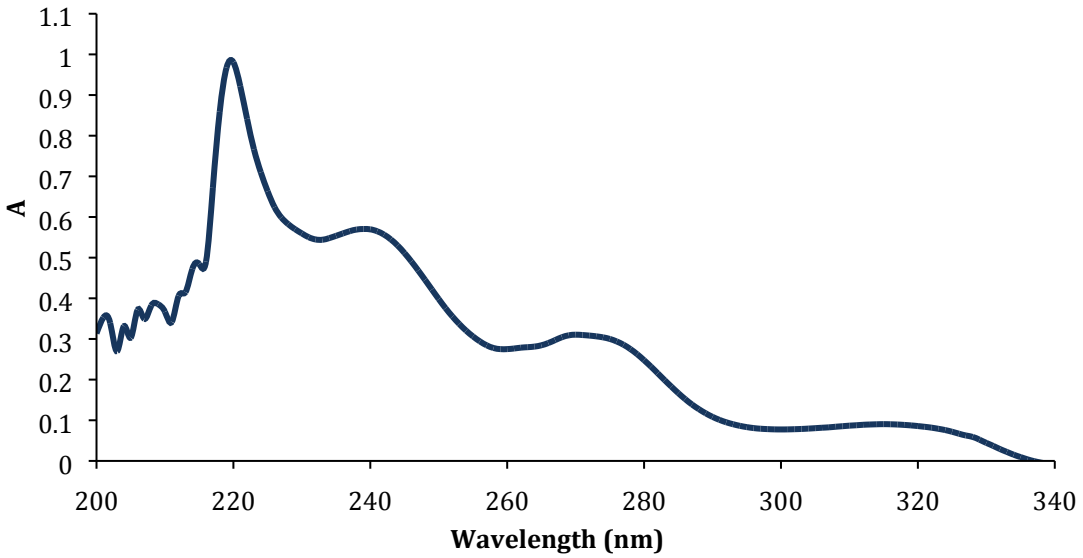

Figure S27: Fluorescence spectra of **GdL^3** (100 μM) in 50:50 MeOH:HEPES buffer (0.1 M; pH = 7.4) in the presence of increasing concentrations (0 to 10 eq.) of Zn^{2+}.