

Supporting Information

Switchable Platinum-based Tweezers with Pt-Pt Bonding and Selective Luminescence Quenching

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NMR spectra of compounds

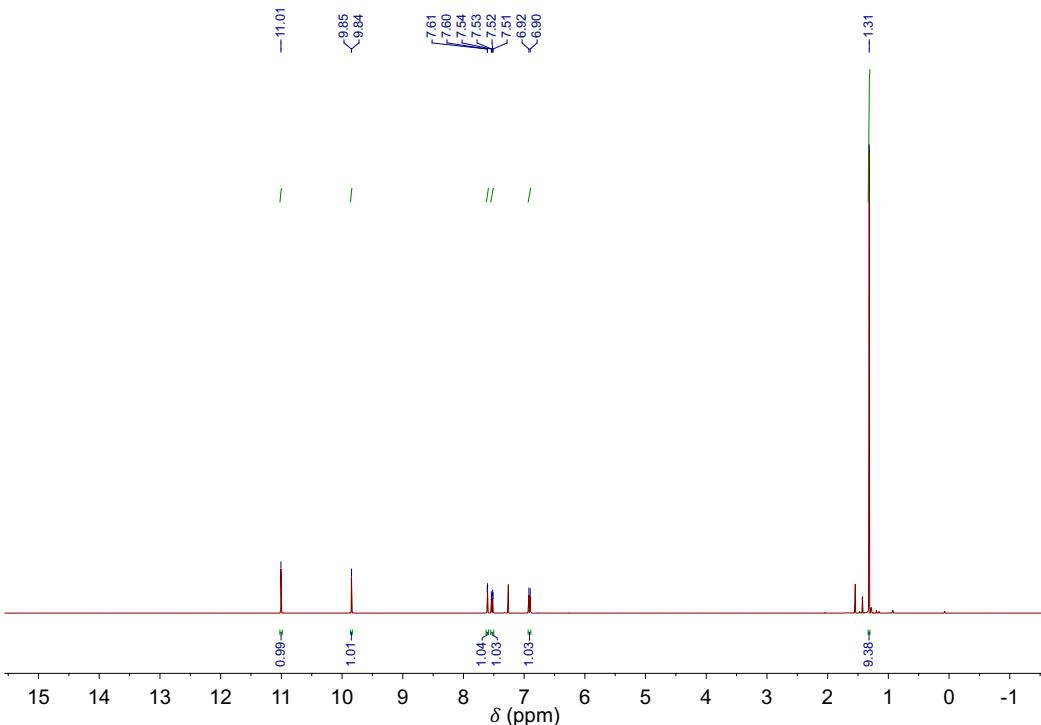


Figure S1. ^1H NMR (400 MHz, 300 K) spectrum of Compound 4 in CDCl_3 .

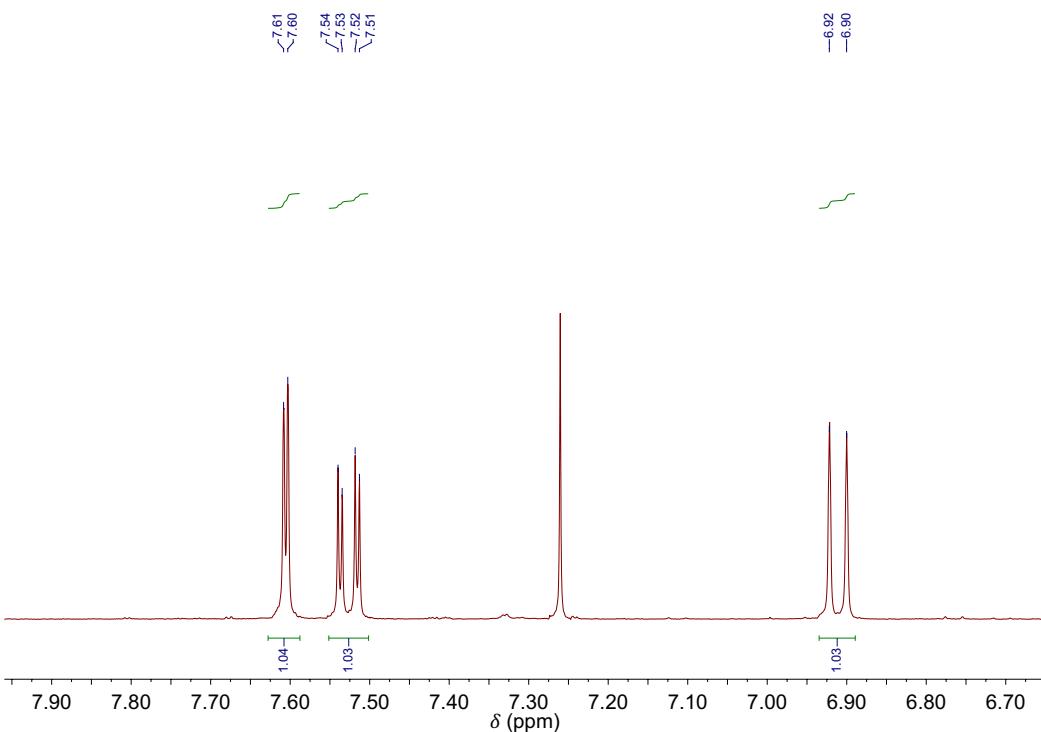


Figure S2. Aromatic region of ^1H NMR (400 MHz, 300 K) spectrum of Compound 4 in CDCl_3 .

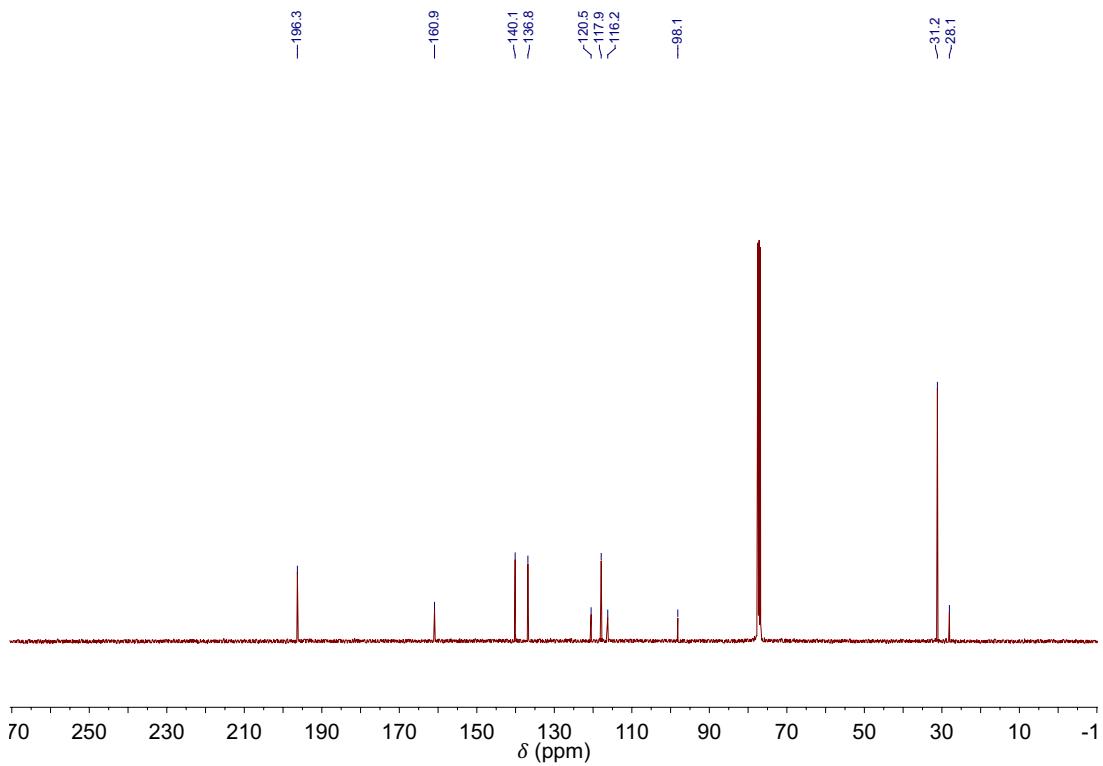


Figure S3. ^{13}C NMR (101 MHz, 300 K) spectrum of Compound 4 in CDCl_3 .

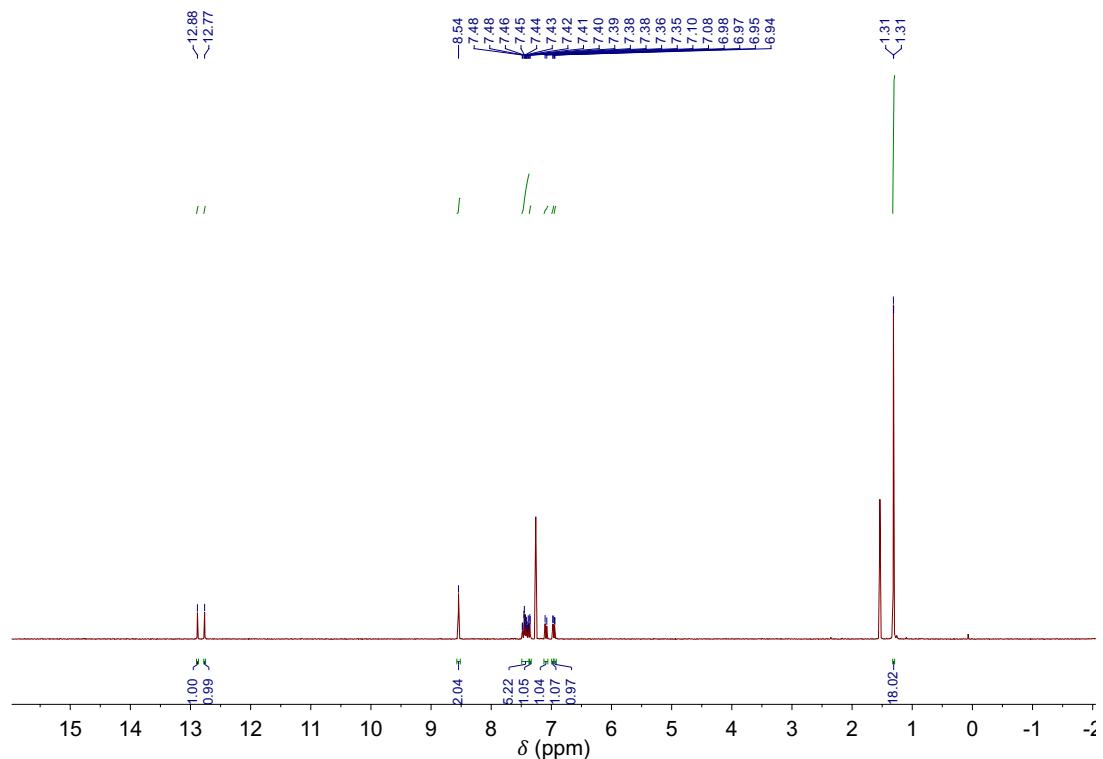


Figure S4. ^1H NMR (400 MHz, 300 K) spectrum of Compound 6 in CDCl_3 .

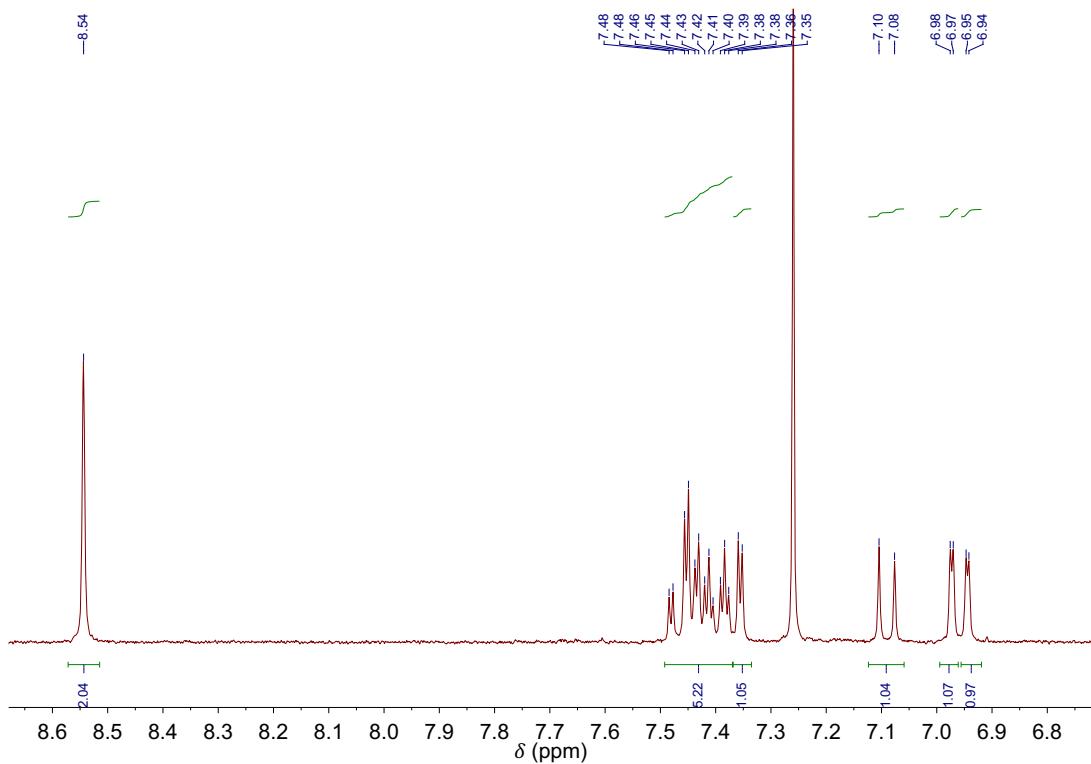


Figure S5. Aromatic region of ^1H NMR (400 MHz, 300 K) spectrum of Compound **6** in CDCl_3 .

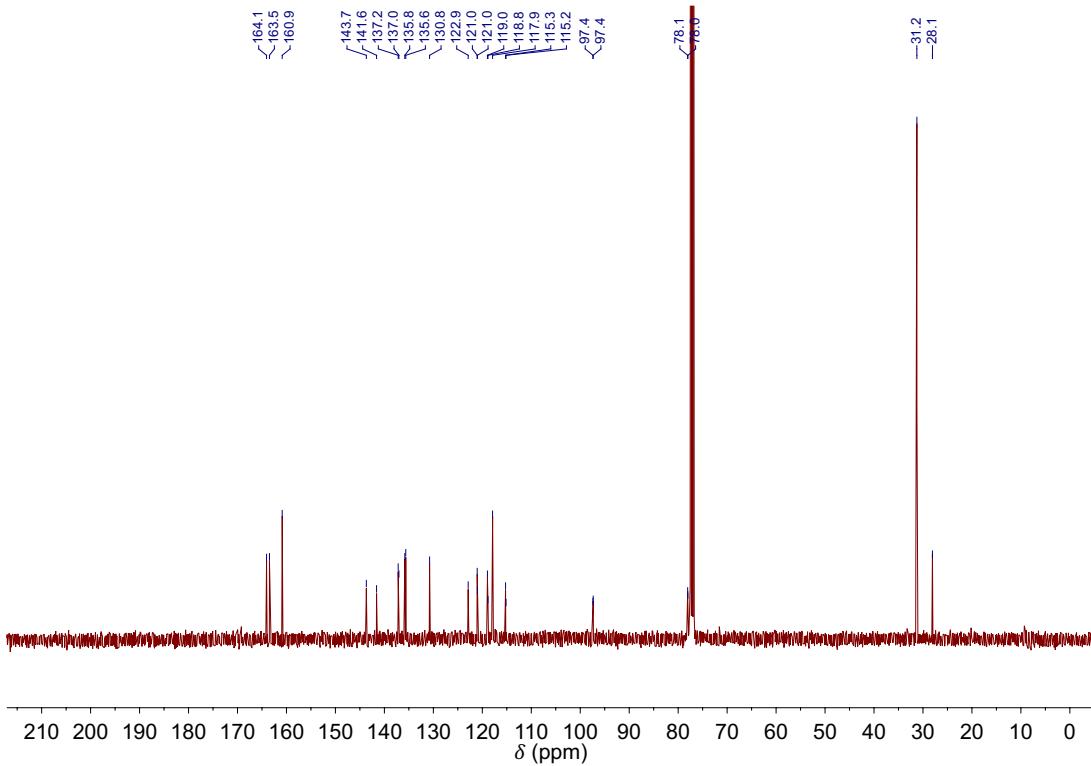


Figure S6. ^{13}C NMR (101 MHz, 300 K) spectrum of Compound **6** in CDCl_3 .

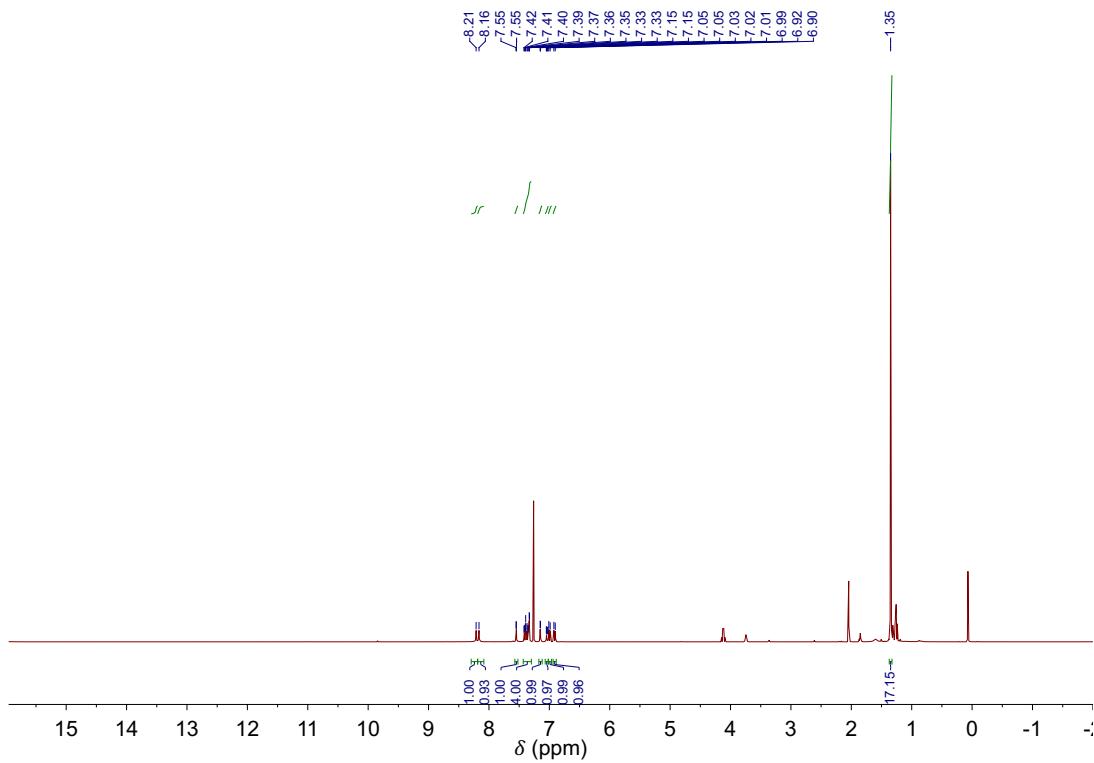


Figure S7. ^1H NMR (400 MHz, 300 K) spectrum of Compound 7 in CDCl_3 .

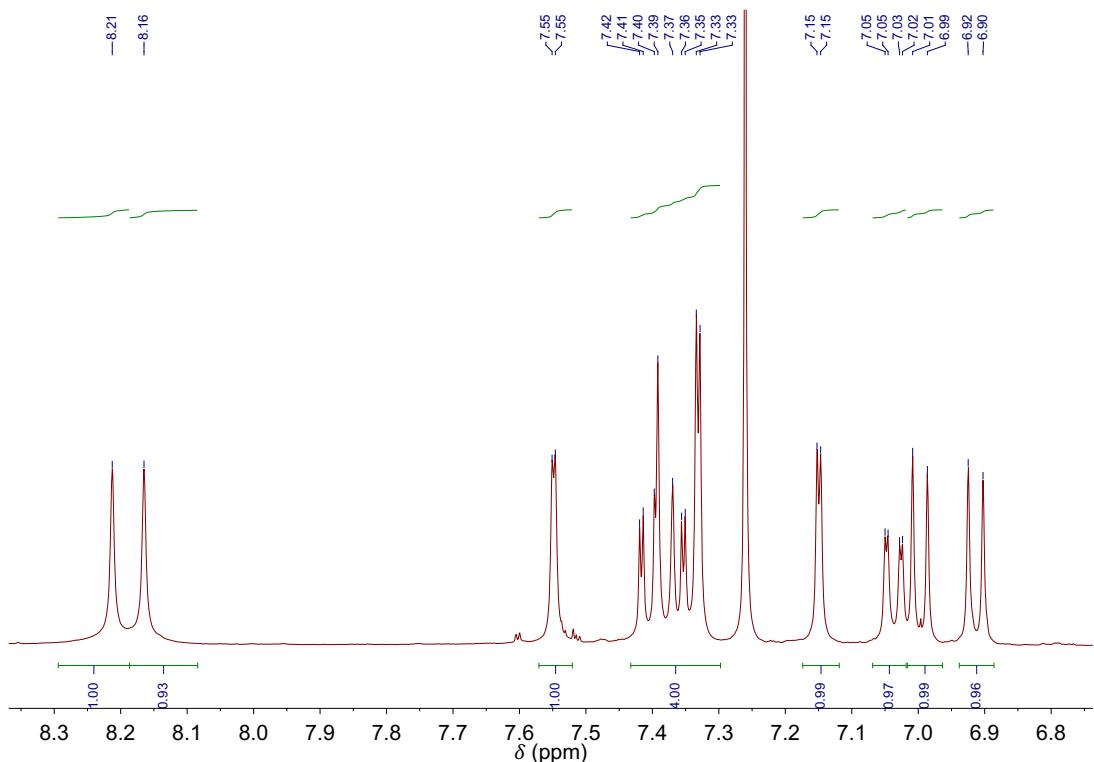


Figure S8. Aromatic region of ^1H NMR (400 MHz, 300 K) spectrum of Compound 7 in CDCl_3 .

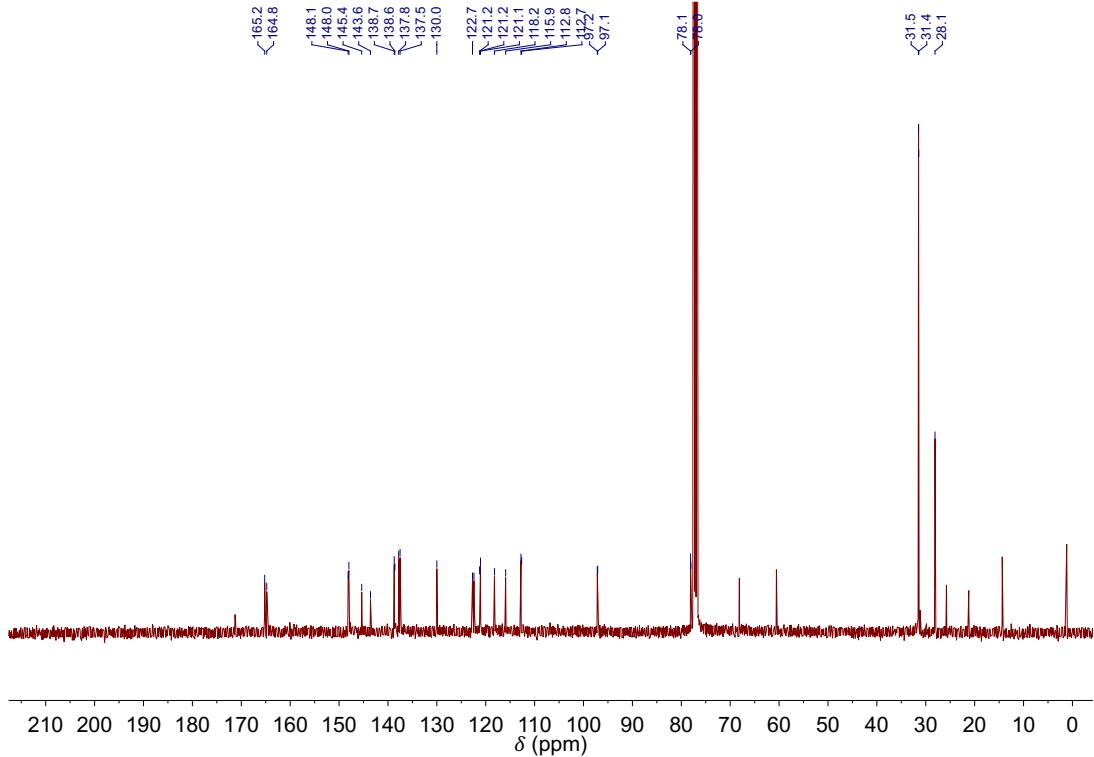


Figure S9. ^{13}C NMR (101 MHz, 300 K) spectrum of Compound **7** in CDCl_3 .

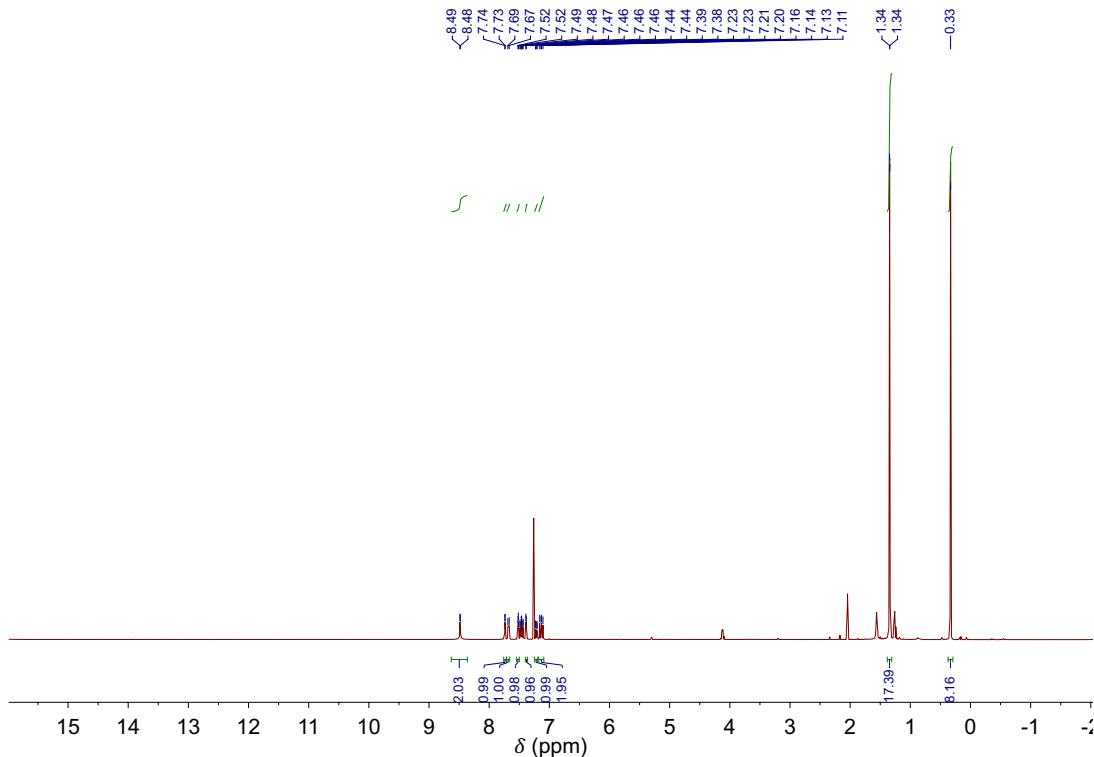


Figure S10. ^1H NMR (400 MHz, 300 K) spectrum of Compound **8** in CDCl_3 .

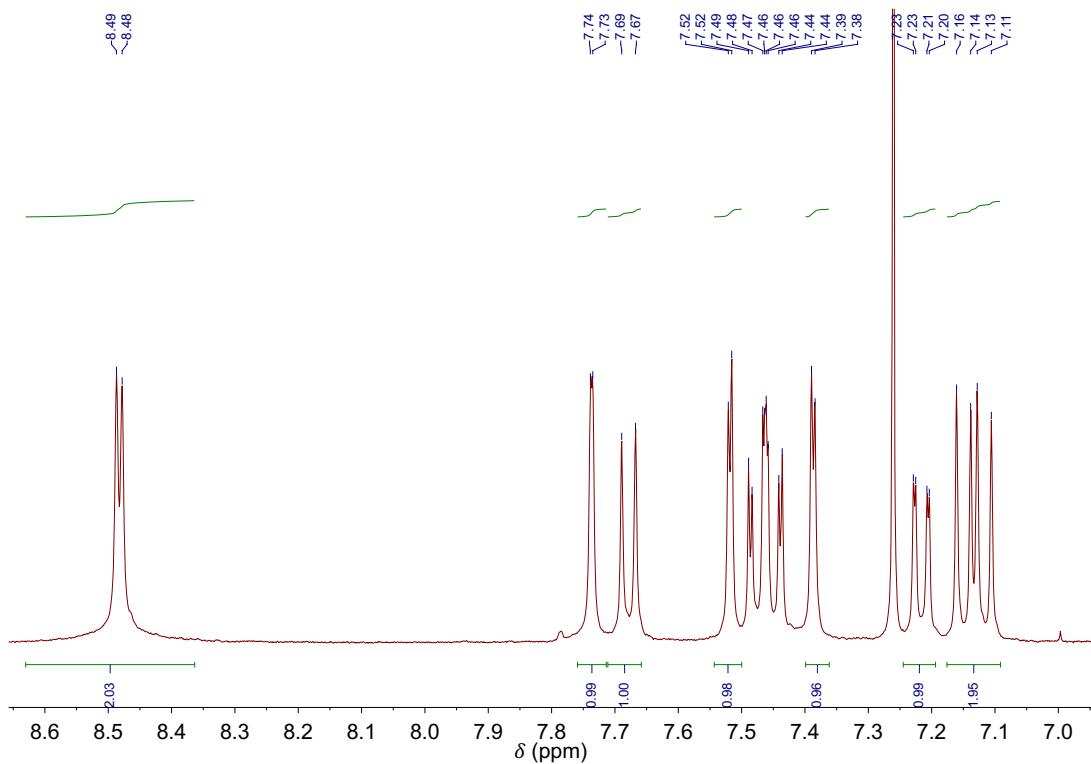


Figure S11. Aromatic region of ^1H NMR (400 MHz, 300 K) spectrum of Compound **8** in CDCl_3 .

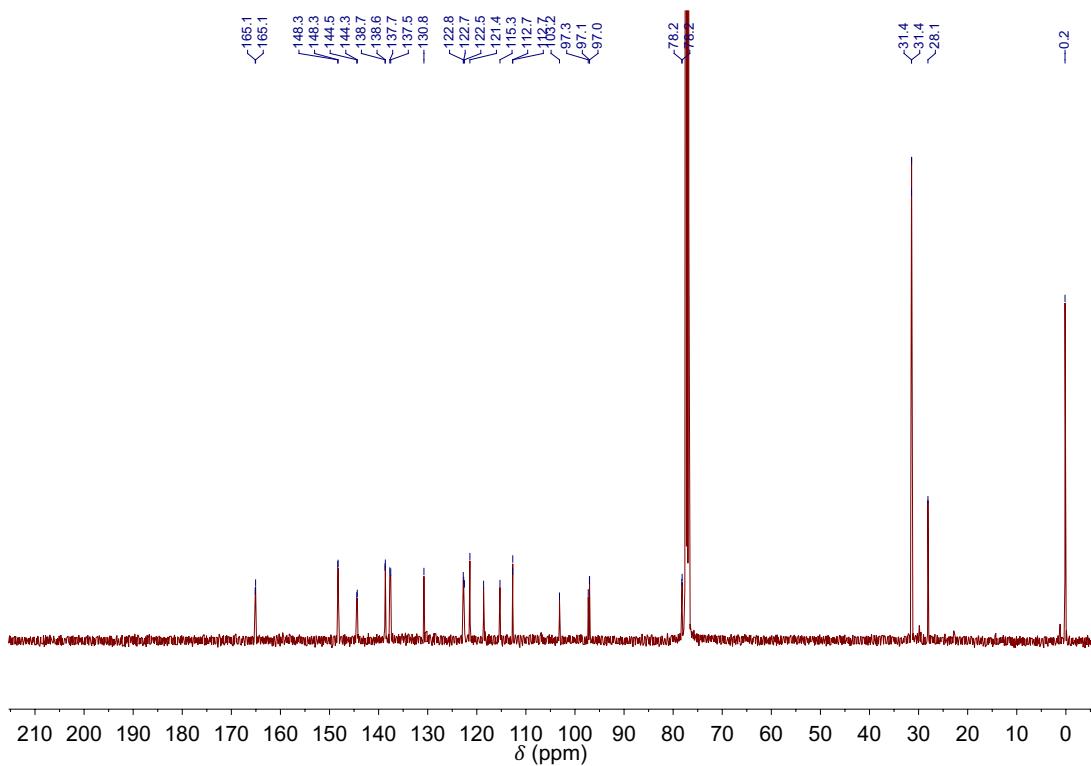


Figure S12. ^{13}C NMR (101 MHz, 300 K) spectrum of Compound **8** in CDCl_3 .

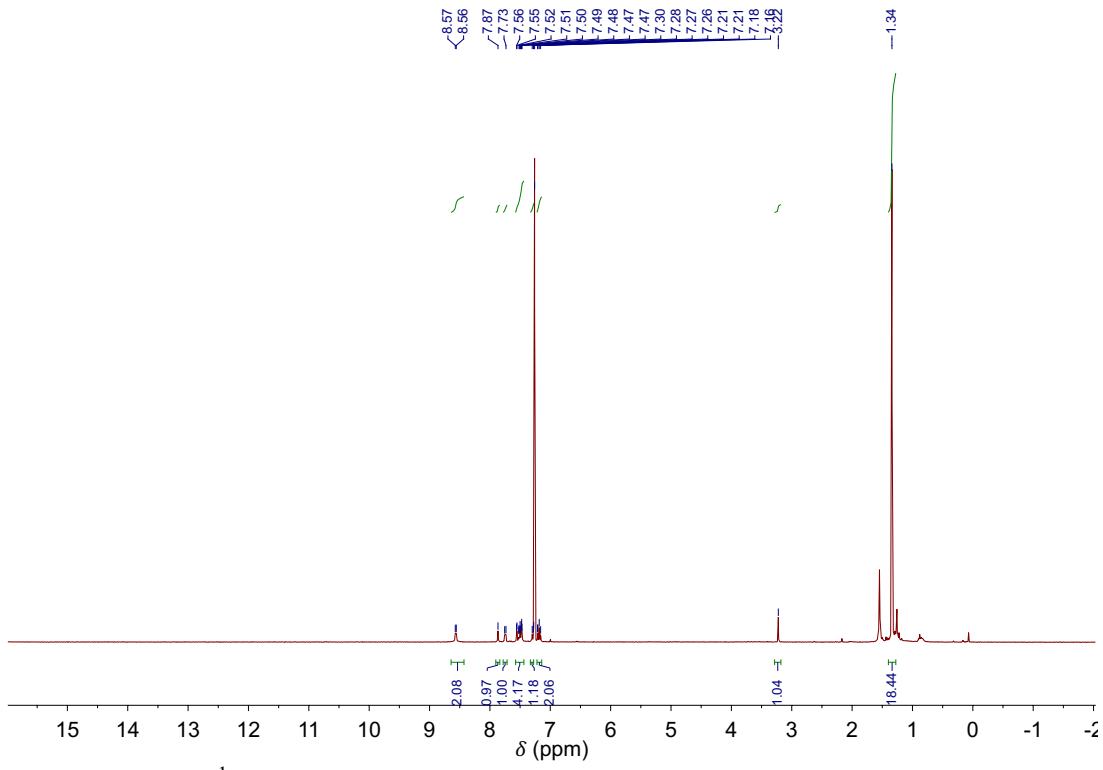


Figure S13. ^1H NMR (400 MHz, 300 K) spectrum of Compound **9** in CDCl_3 .

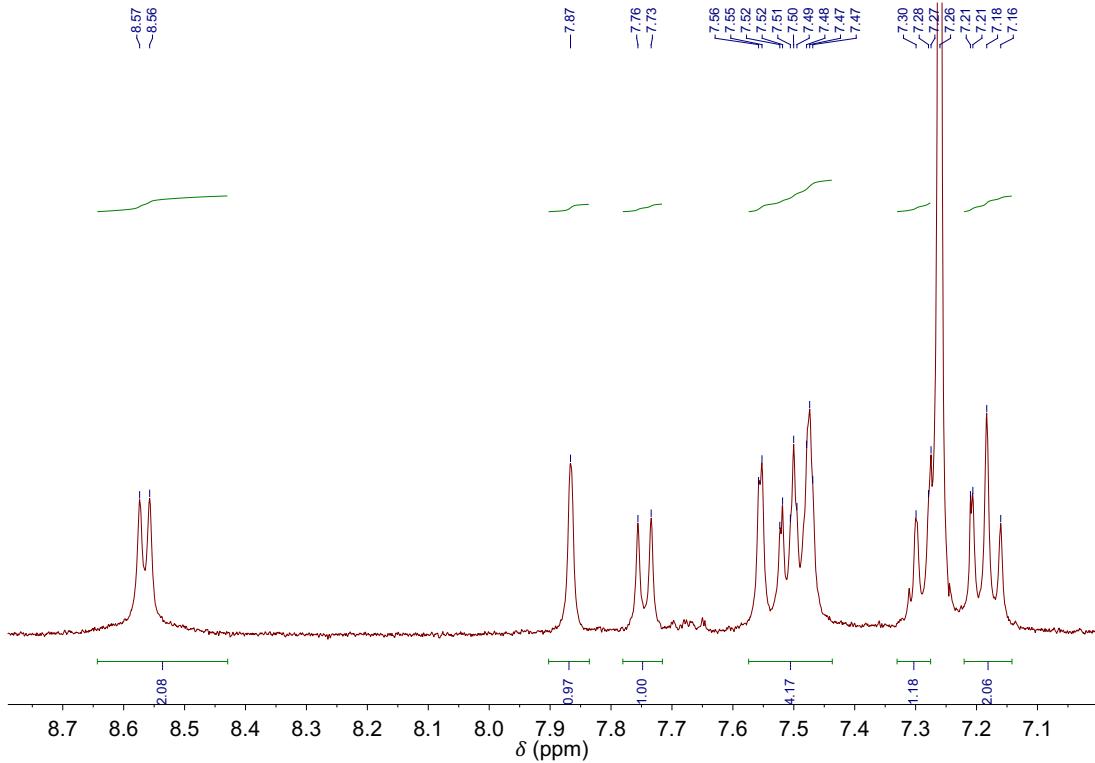


Figure S14. Aromatic region of ^1H NMR (400 MHz, 300 K) spectrum of Compound **9** in CDCl_3 .

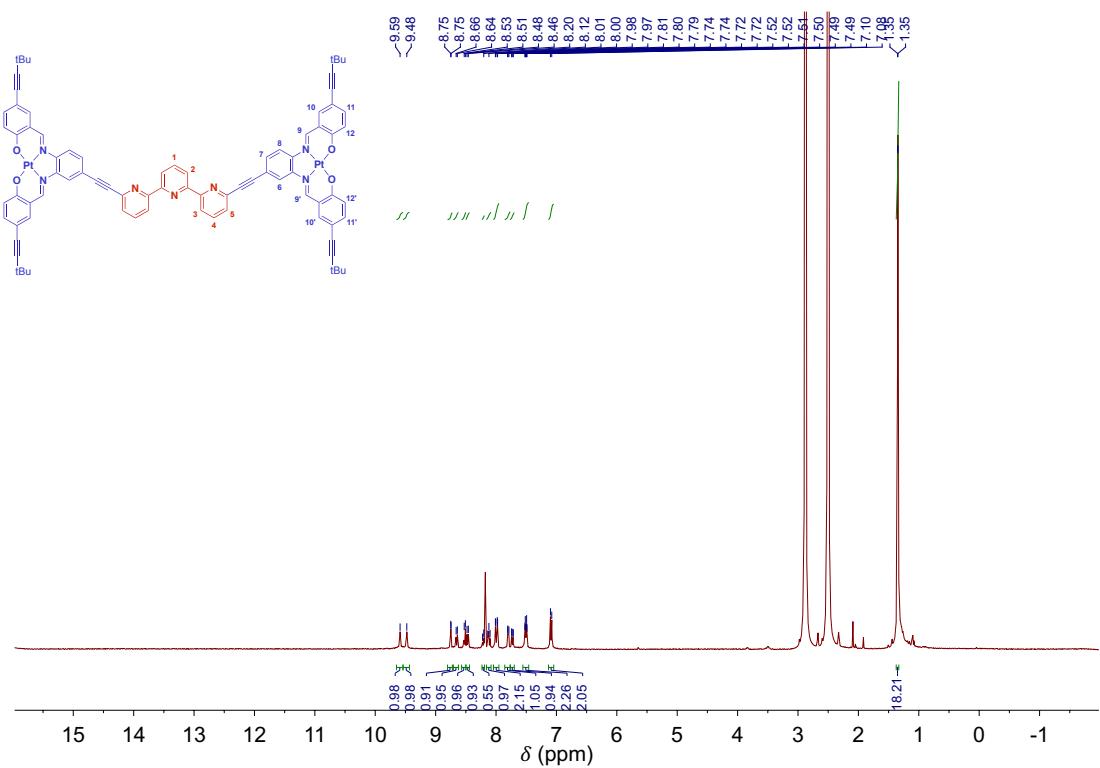


Figure S15. ^1H NMR (400 MHz, 370 K) spectrum of Tweezers **1** in $\text{DMSO}-d_6$.

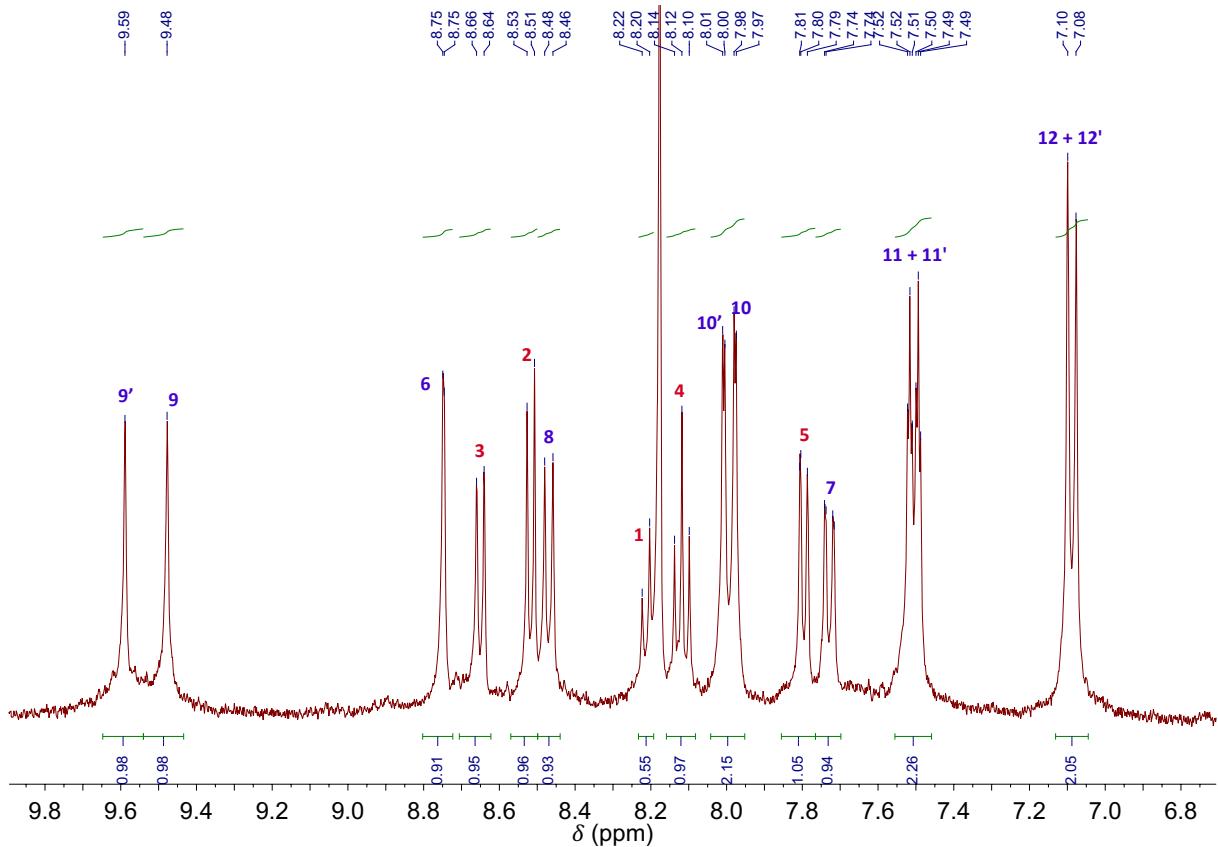


Figure S16. Aromatic region of ^1H NMR (400 MHz, 370 K) spectrum of Tweezers **1** in $\text{DMSO}-d_6$.

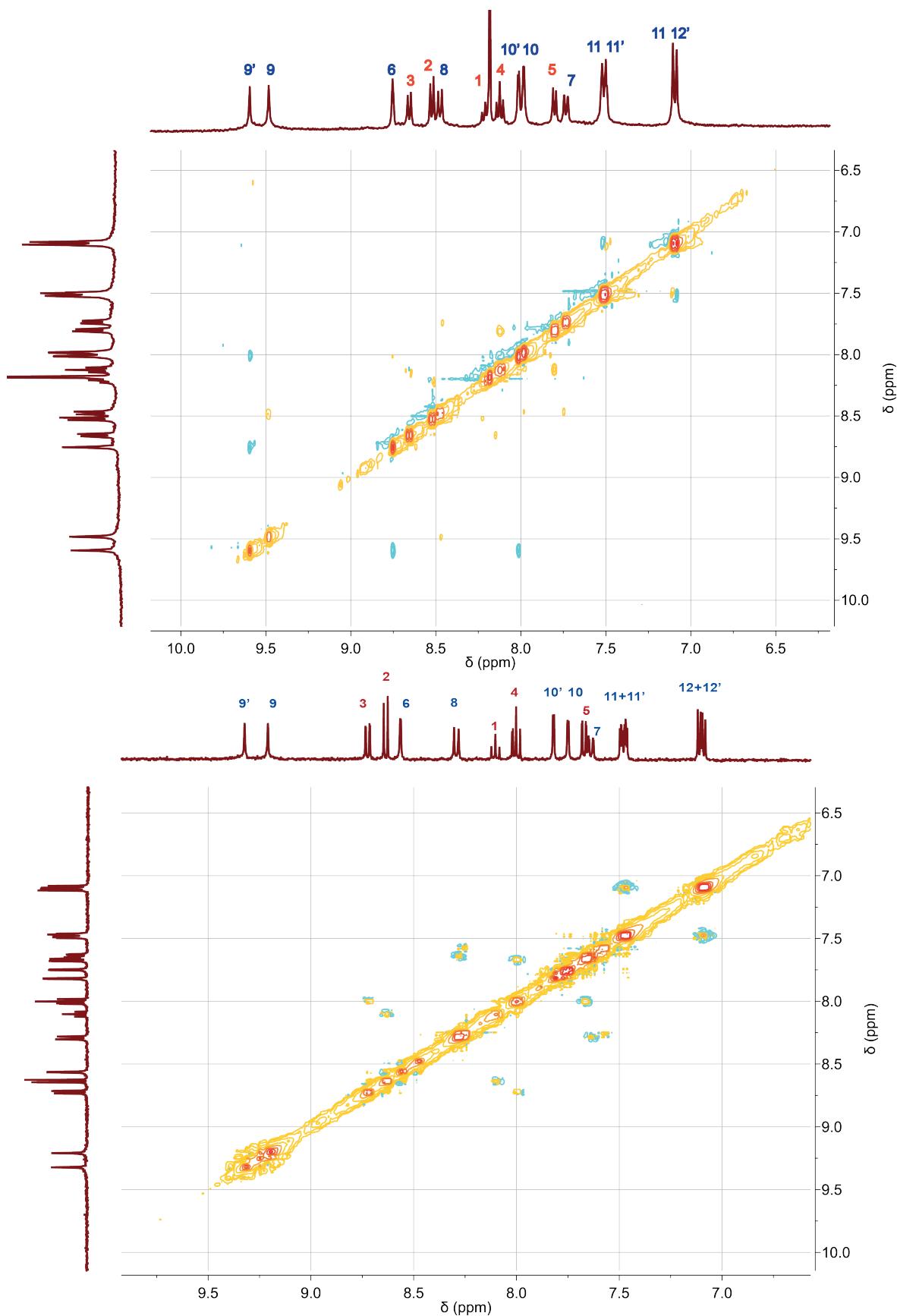


Figure S17 NOESY (400 MHz) spectrum of Tweezers **1** in $\text{DMSO}-d_6$ at 370 K (top) and $\text{THF}-d_8$ at 300K (bottom).

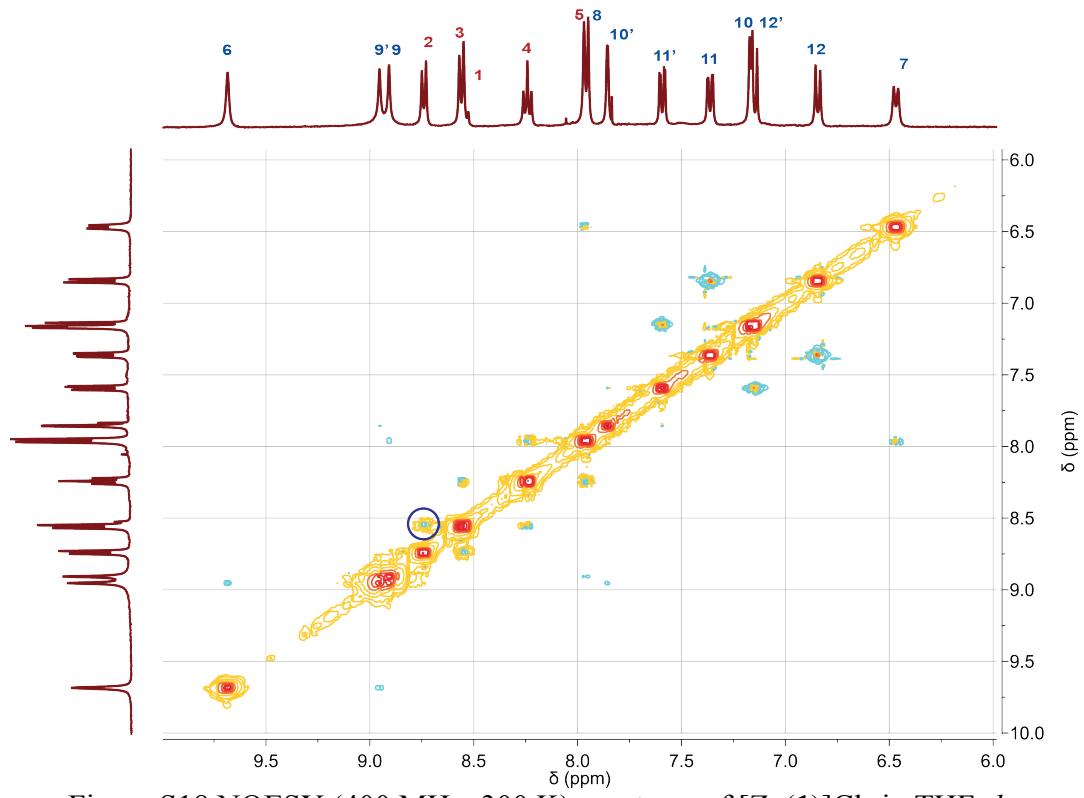


Figure S18 NOESY (400 MHz, 300 K) spectrum of $[\text{Zn}(\mathbf{1})]\text{Cl}_2$ in $\text{THF}-d_8$.

Mass spectra of 1

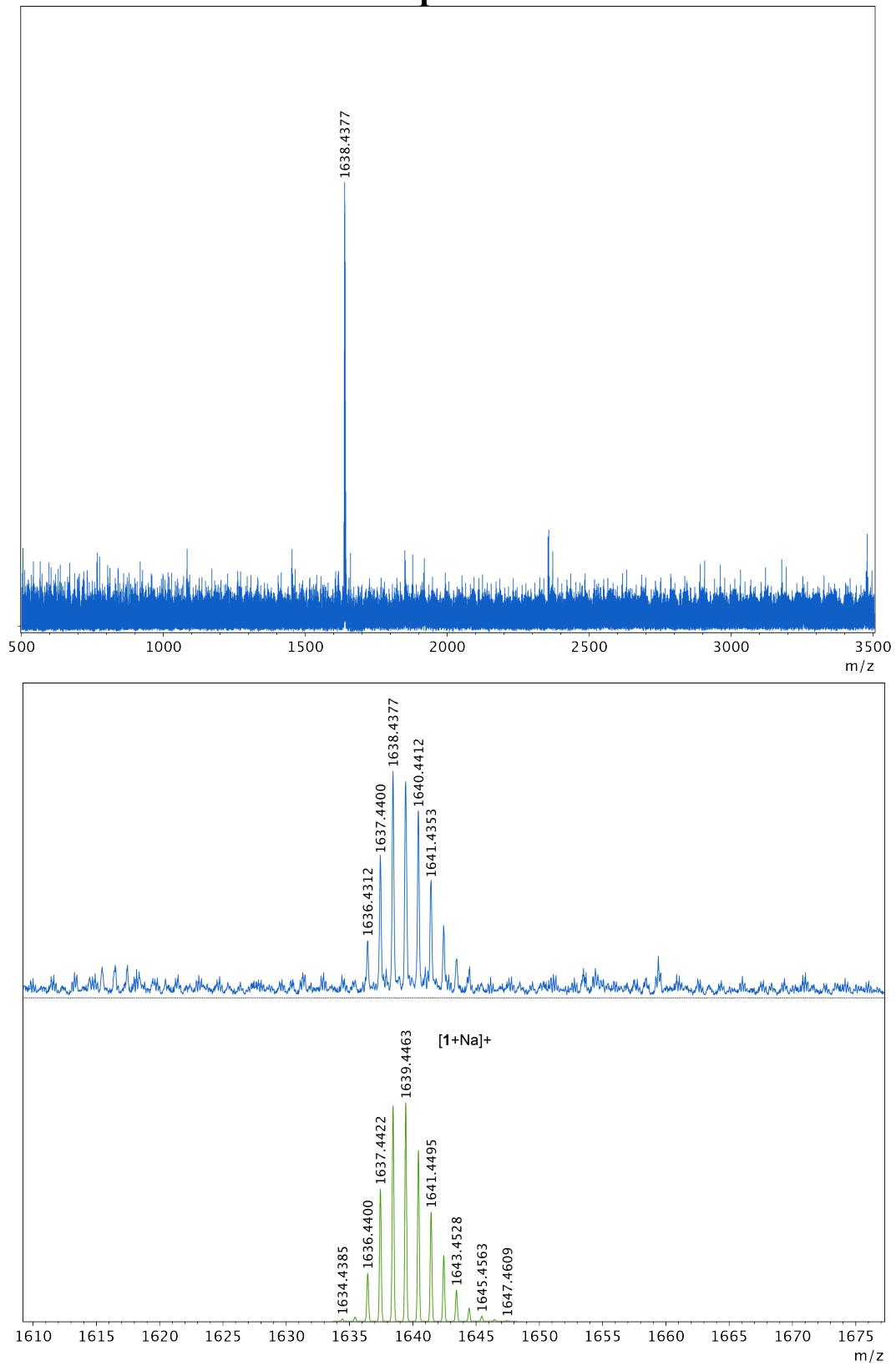


Figure S19 ESI-TOF HRMS spectra of tweezers **1** and isotopic pattern experimental (top) and calculated (bottom).

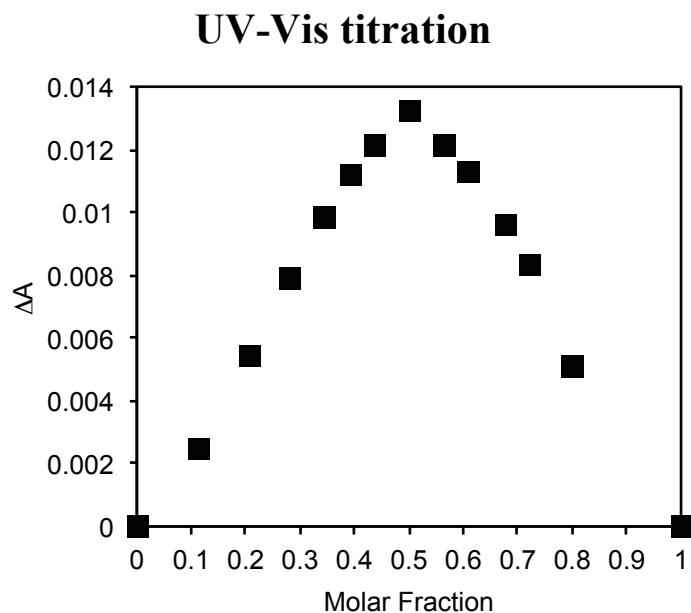


Figure S20. Job plot of Tweezers **1** with $Zn(ClO_4)_2$ at 600 nm showing the formation of the 1:1 complex $[Zn(\mathbf{1})]^{2+}$.

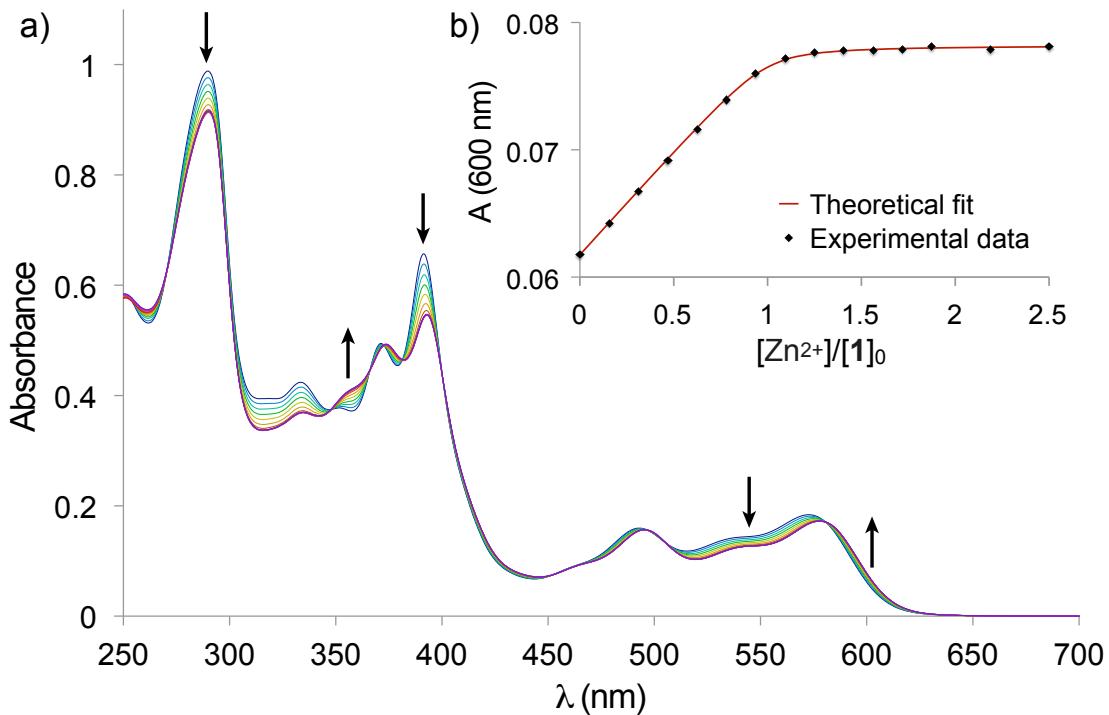


Figure S21. a) UV-Vis titration of tweezers **1** (5.0×10^{-6} mol.L⁻¹) upon addition of ZnCl₂ in THF. b) Absorbance at 600 nm and 1:1 binding model fit.

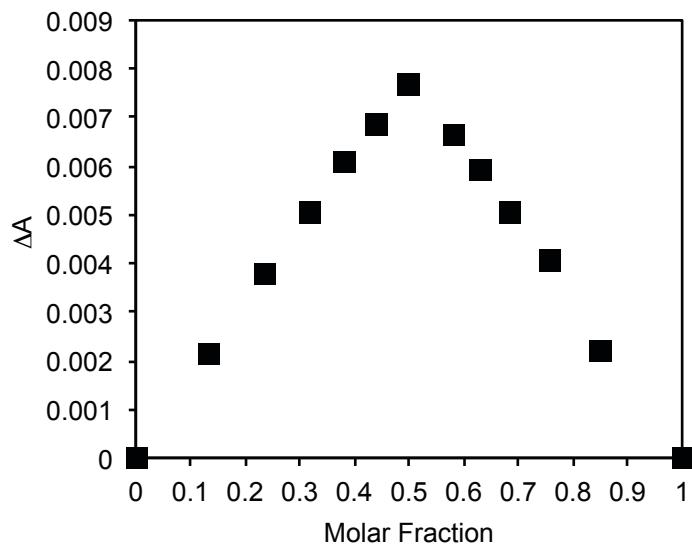


Figure S22. Job plot of Tweezers **1** with ZnCl₂ at 600 nm showing the formation of the 1:1 complex $[\text{Zn}(\mathbf{1})]^{2+}$.

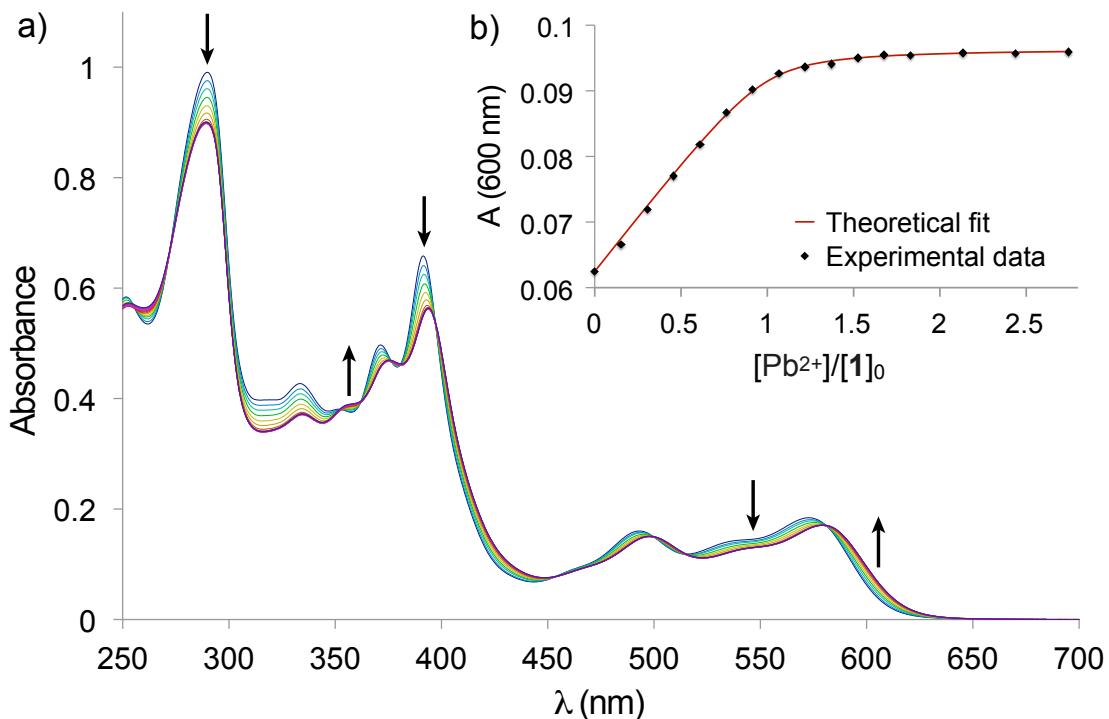


Figure S23. a) UV-Vis titration of tweezers **1** (5.0×10^{-6} mol.L⁻¹) upon addition of Pb(ClO₄)₂ in THF. b) Absorbance at 600 nm and 1:1 binding model fit.

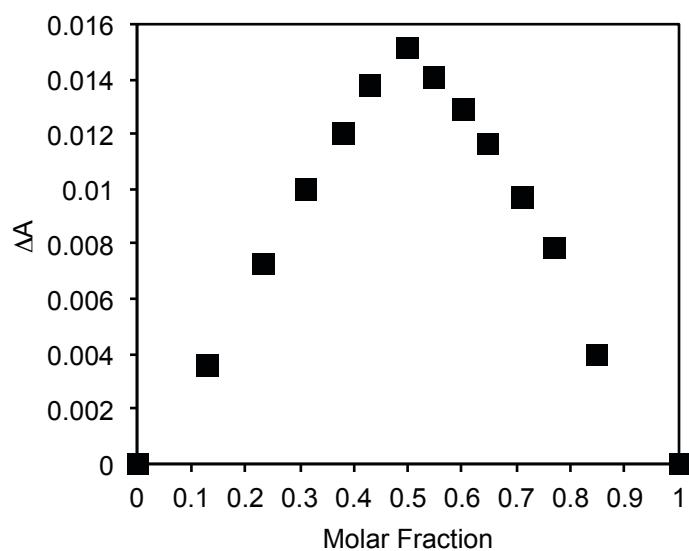


Figure S24. Job plot of Tweezers **1** with Pb(ClO₄)₂ at 600 nm showing the formation of the 1:1 complex [Pb(**1**)]²⁺.

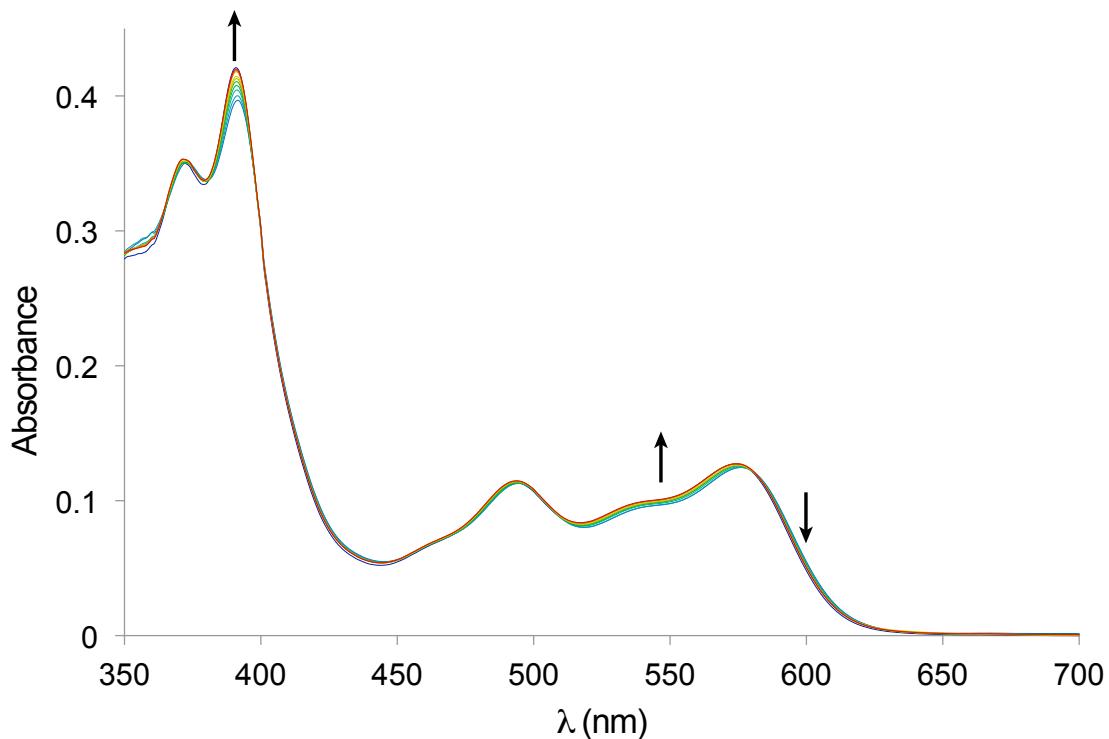


Figure S25. UV-Vis titration of complex $[Zn(1)]^{2+}$ ($5.0 \times 10^{-6} \text{ mol.L}^{-1}$) upon addition of phen (1,10-phenanthroline) in THF.

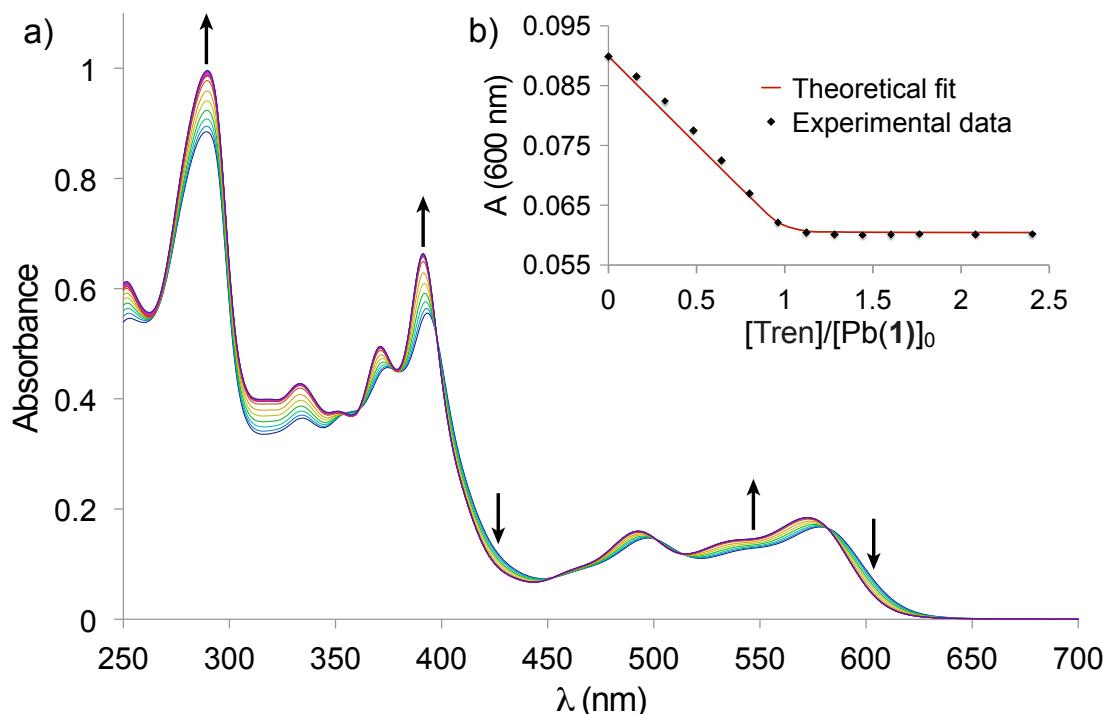


Figure S26. a) UV-Vis titration of complex $[Pb(1)]^{2+}$ ($5.0 \times 10^{-6} \text{ mol.L}^{-1}$) upon addition of tren in THF. b) Absorbance at 600 nm and 1:1 binding model fit.

UV-Vis titration of tweezers **1** with $\text{Hg}(\text{ClO}_4)_2$: Closing and intercalation

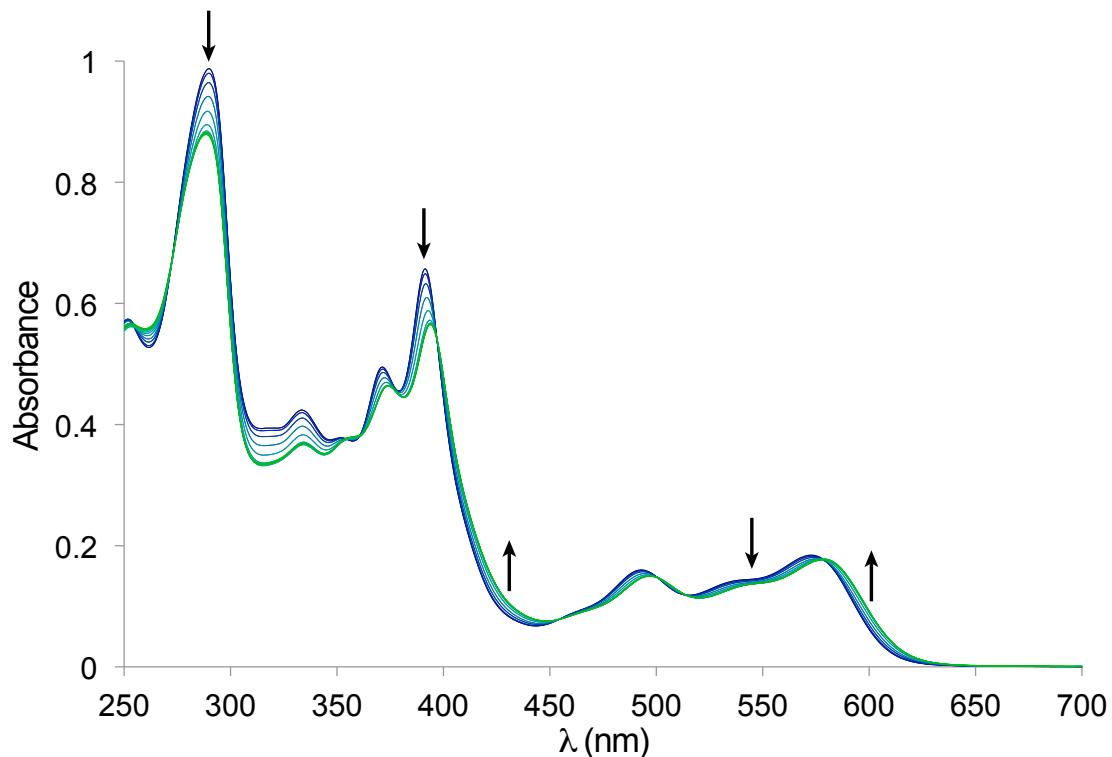


Figure S27. UV-Vis titration of tweezers **1** (5.0×10^{-6} mol.L $^{-1}$) upon addition of $\text{Hg}(\text{ClO}_4)_2$ in THF, from 0 to 1 equivalents.

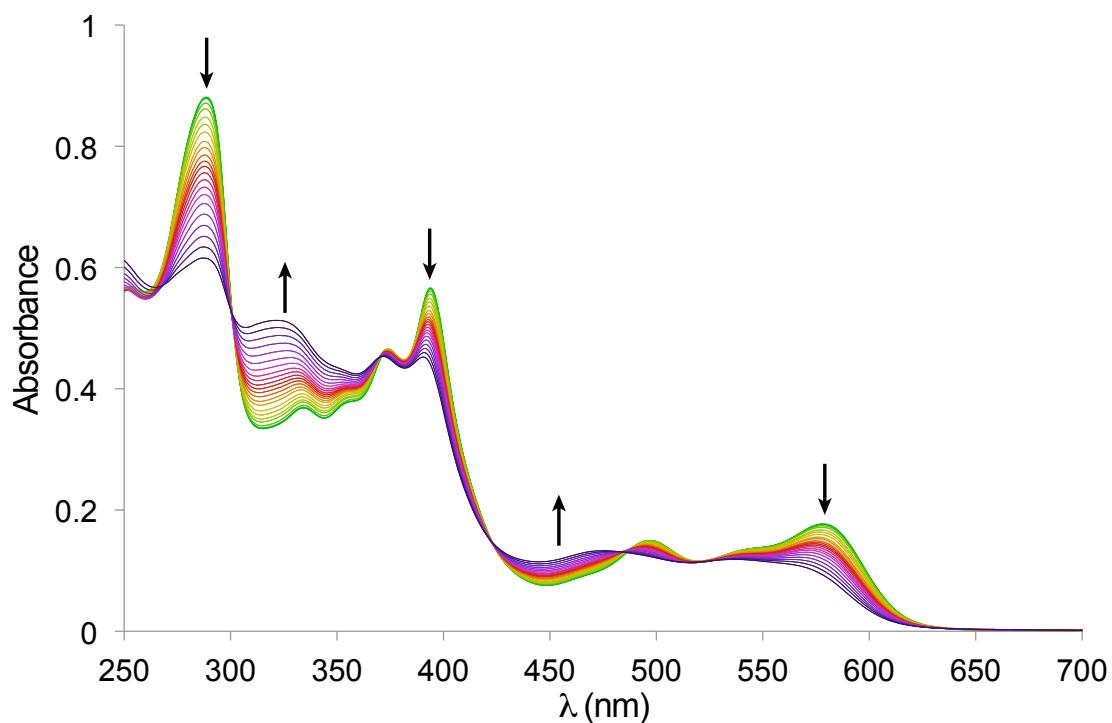


Figure S28. UV-Vis titration of tweezers **1** (5.0×10^{-6} mol.L $^{-1}$) upon addition of $\text{Hg}(\text{ClO}_4)_2$ in THF, from 1 to 10 equivalent.

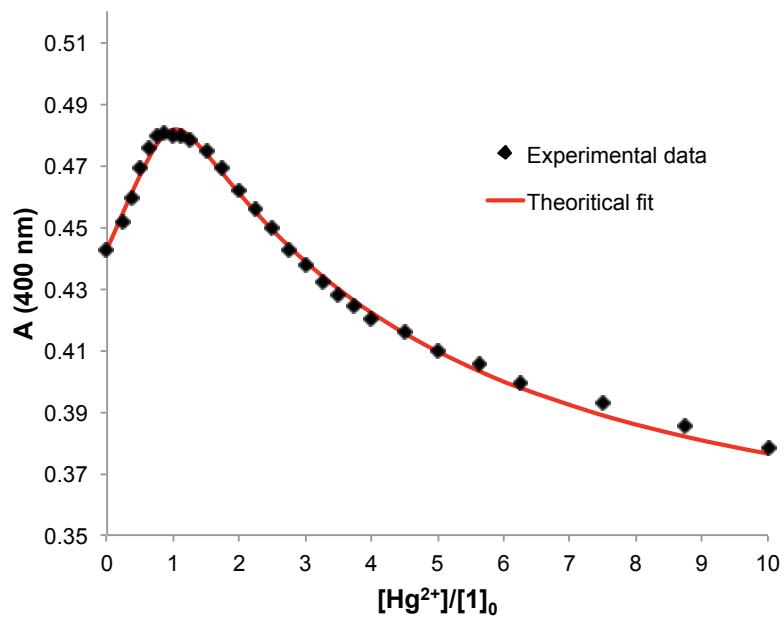


Figure S29 Absorbance at 400 nm of the titration of **1** with Hg²⁺ and 1:2 binding model fit.

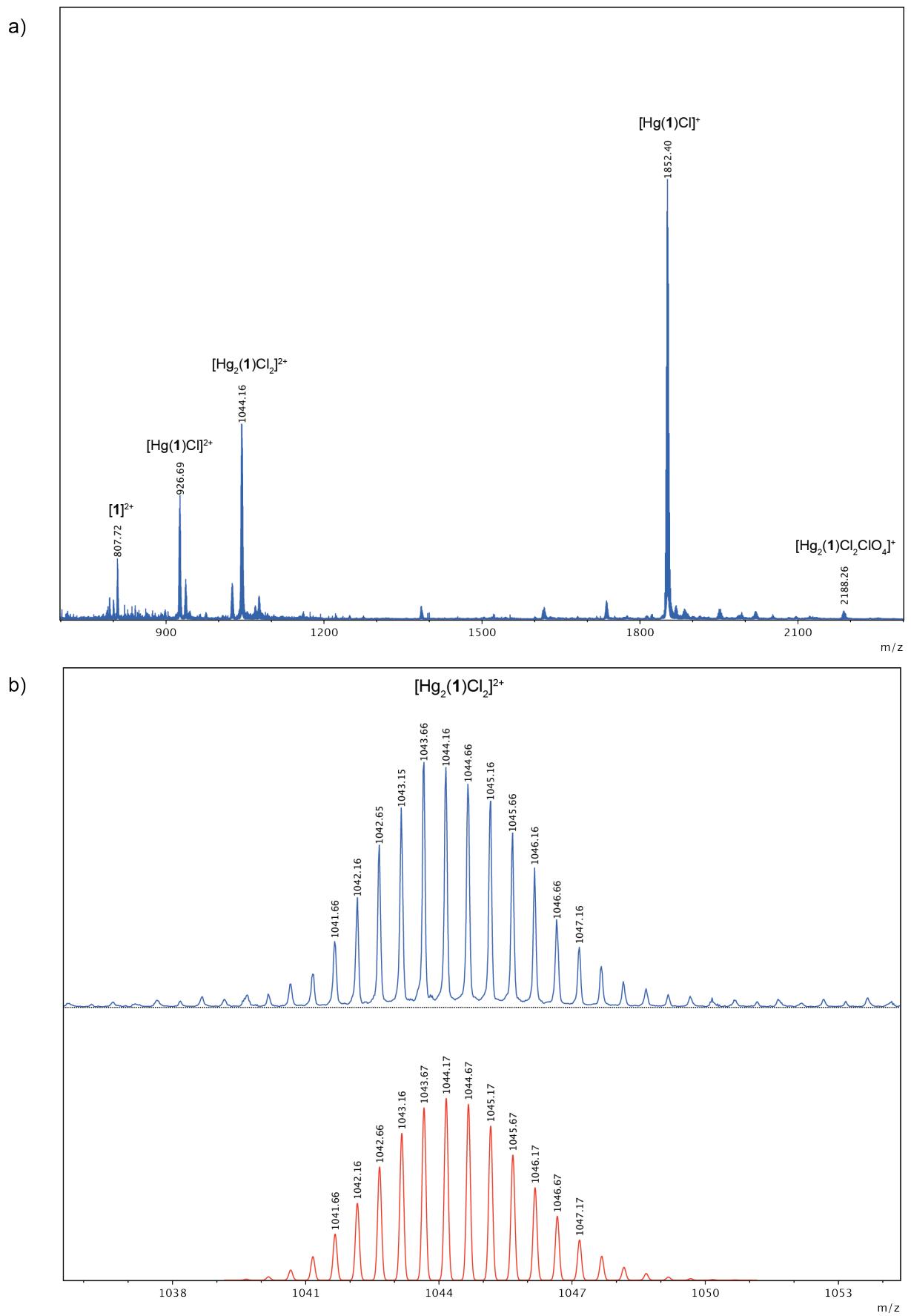


Figure S30 a) Full mass spectra (ESI-Tof) of $[\text{Hg}_2(1)]^{4+}$ b) experimental isotopic pattern (top) and calculated (bottom) for $[\text{Hg} \subset \text{Hg}(1)\text{Cl}_2]^{2+}$.

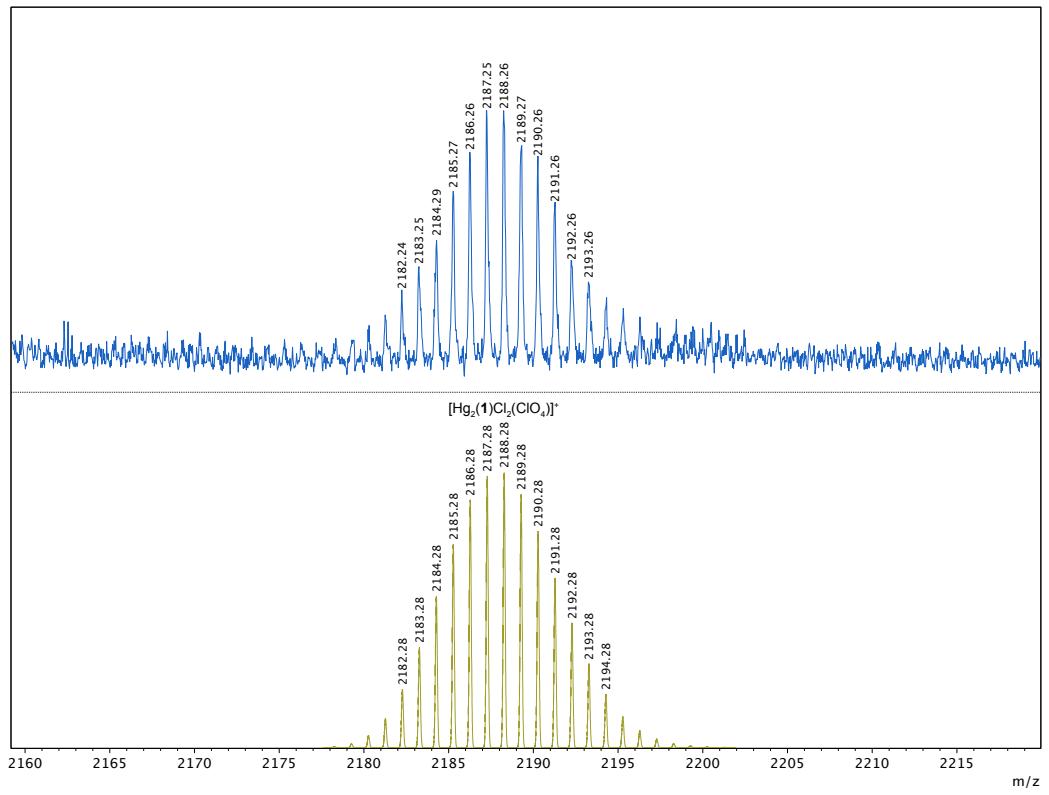


Figure S31 Experimental (top) and calculated (bottom) isotopic pattern for $[Hg(ClO_4) \subset Hg(1)Cl_2]^+$.

Emission spectra and solvatochromism

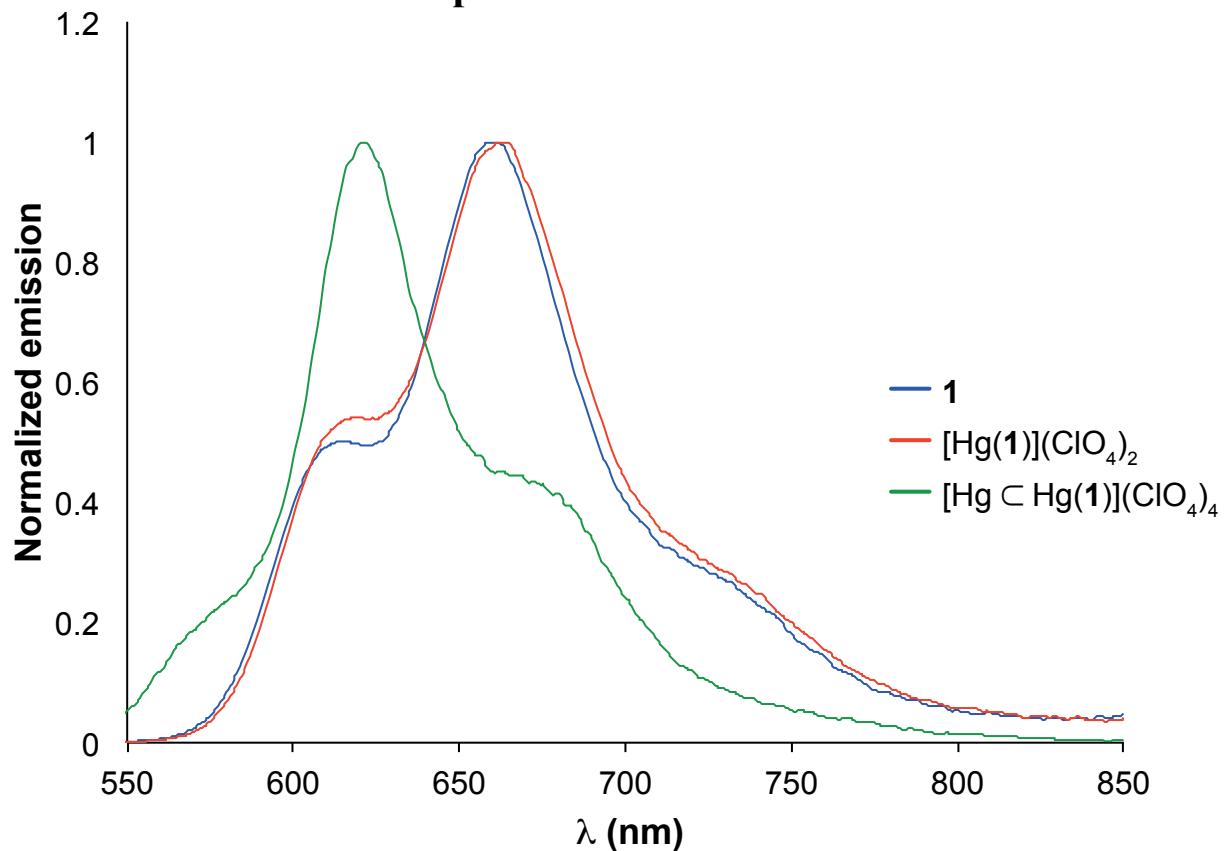


Figure S32 Normalized emission spectra in THF at 298 K ($\lambda_{ex} = 532$ nm).

Conc. 5.0×10^{-6} mol.L⁻¹.

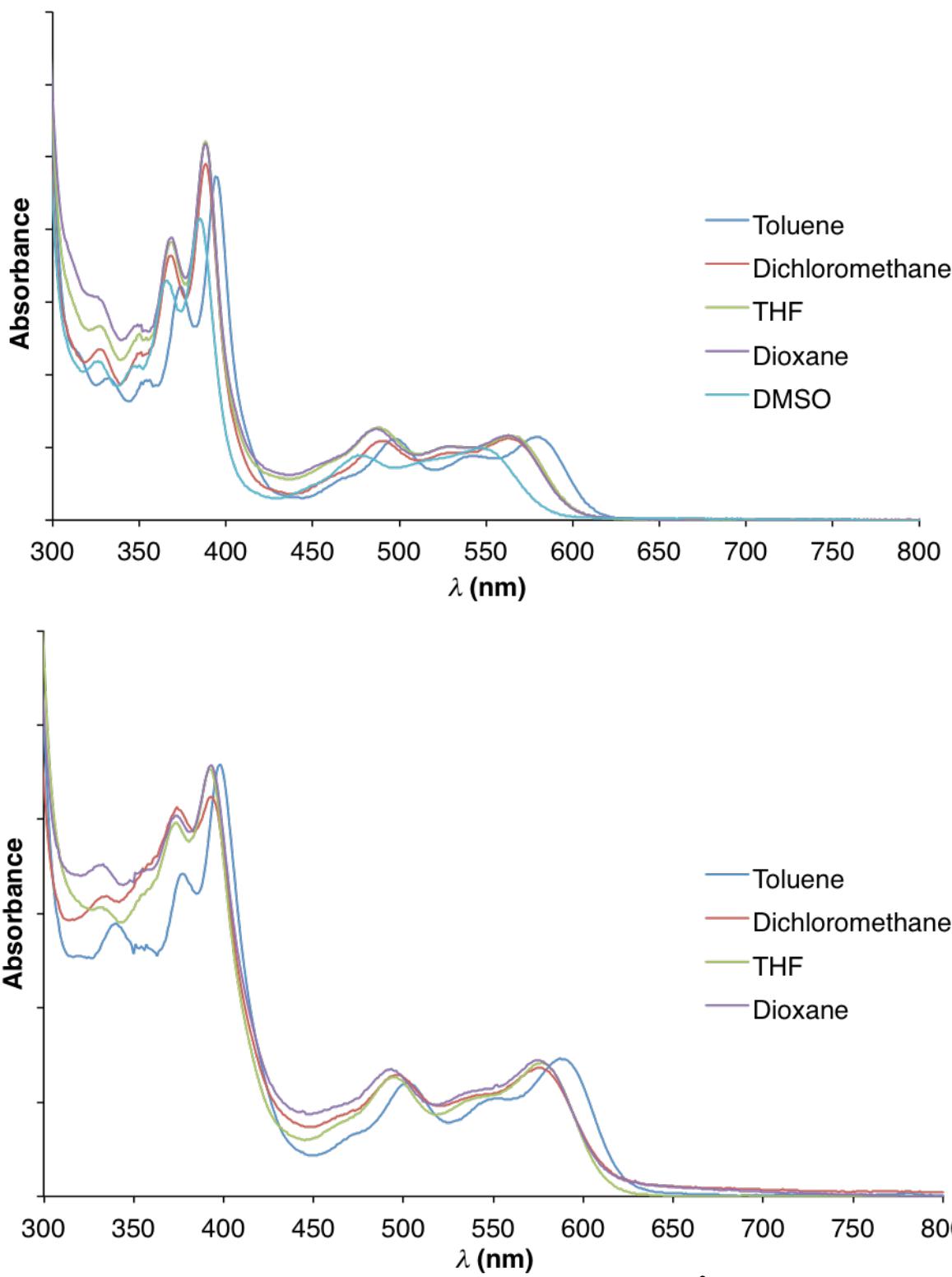


Figure S33 Electronic absorption spectra of **8** (top) and $[Zn(1)]^{2+}$ (bottom) in different solvents at $5.0 \times 10^{-6} \text{ mol.L}^{-1}$. Spectra are normalised with respect to lowest energy absorption band.

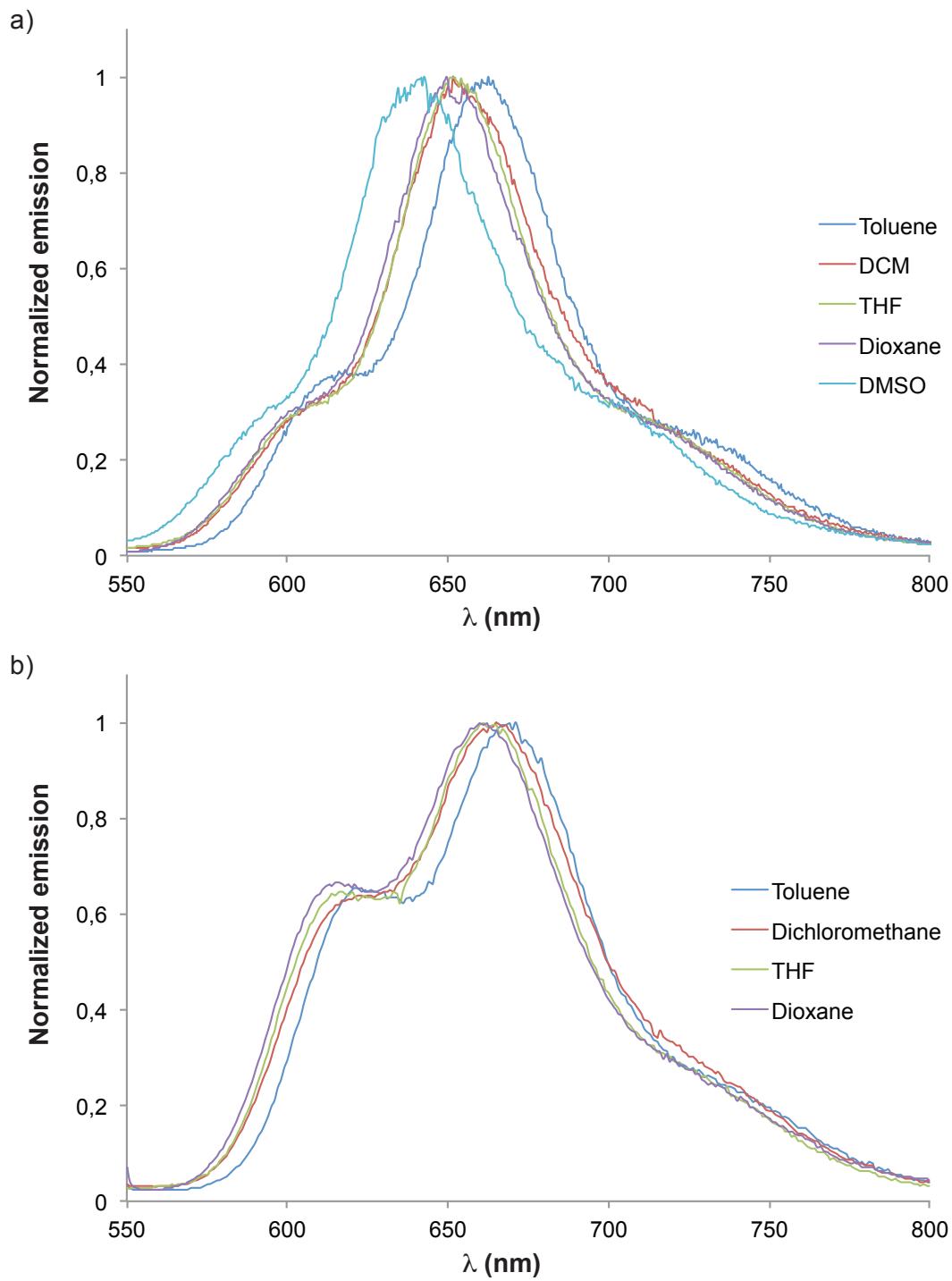


Figure S34 Normalized emission spectra of a) **8** and b) $[\text{Zn(1)}]^{2+}$ in different solvents at $5.0 \times 10^{-6} \text{ mol.L}^{-1}$ ($\lambda_{ex} = 532 \text{ nm}$).

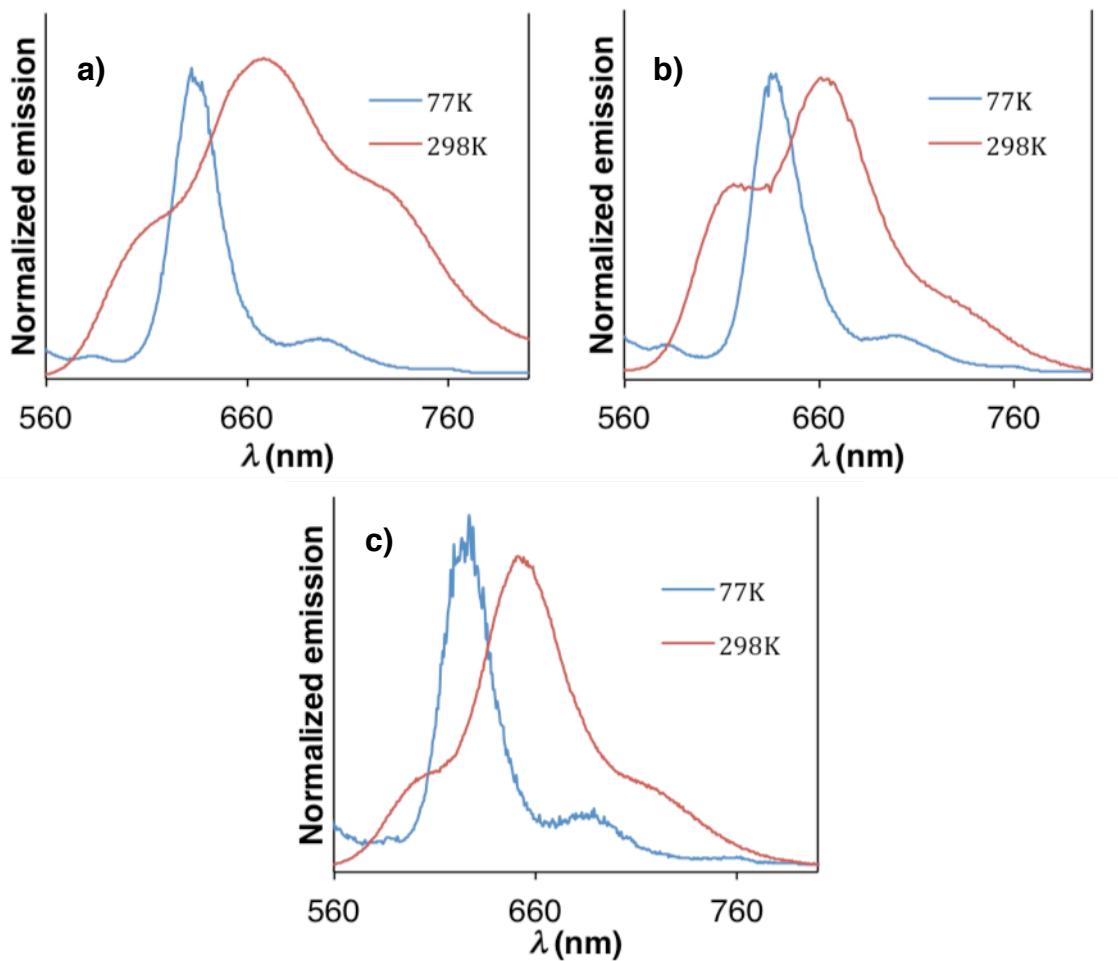


Figure S35 Normalized emission spectra of a) **1**; b) $[\text{Zn}(\mathbf{1})]^{2+}$ and c) **8** in THF at 298 K and 2-MeTHF at 77 K ($\lambda_{\text{ex}} = 532 \text{ nm}$). Conc. $5.0 \times 10^{-6} \text{ mol.L}^{-1}$.