Electronic Supplementary Information

A Ru(II)-Arene-Ferrocene Complex With Promising Antibacterial Activity

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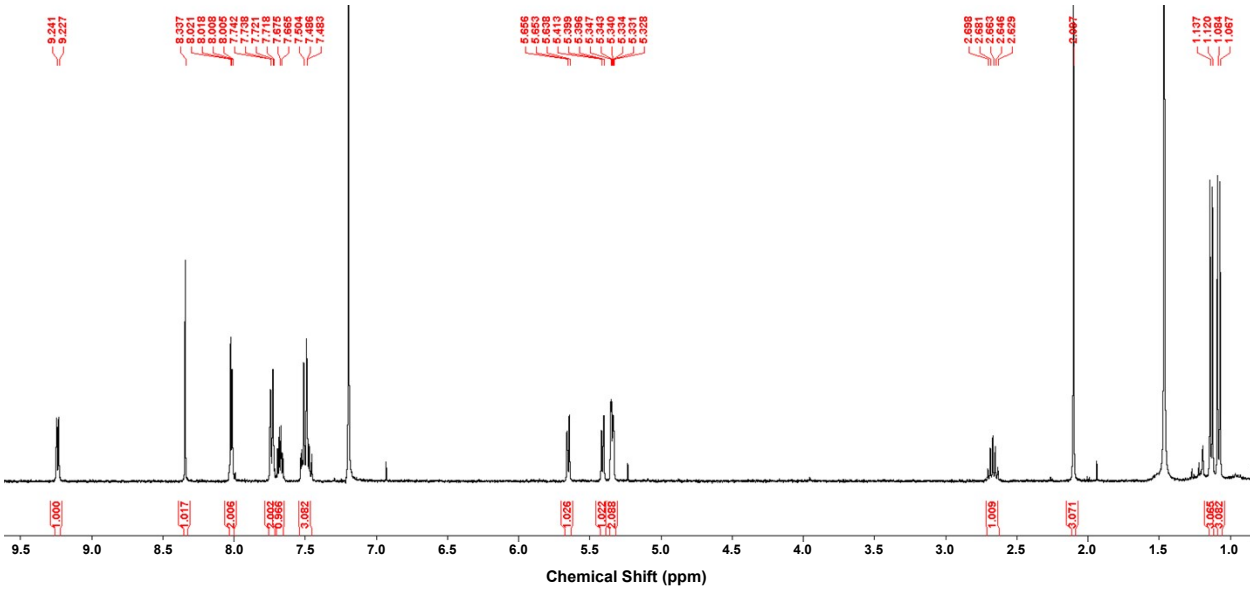

Figure S1. ^{1}H NMR of **C1** in $CDCl_3$.

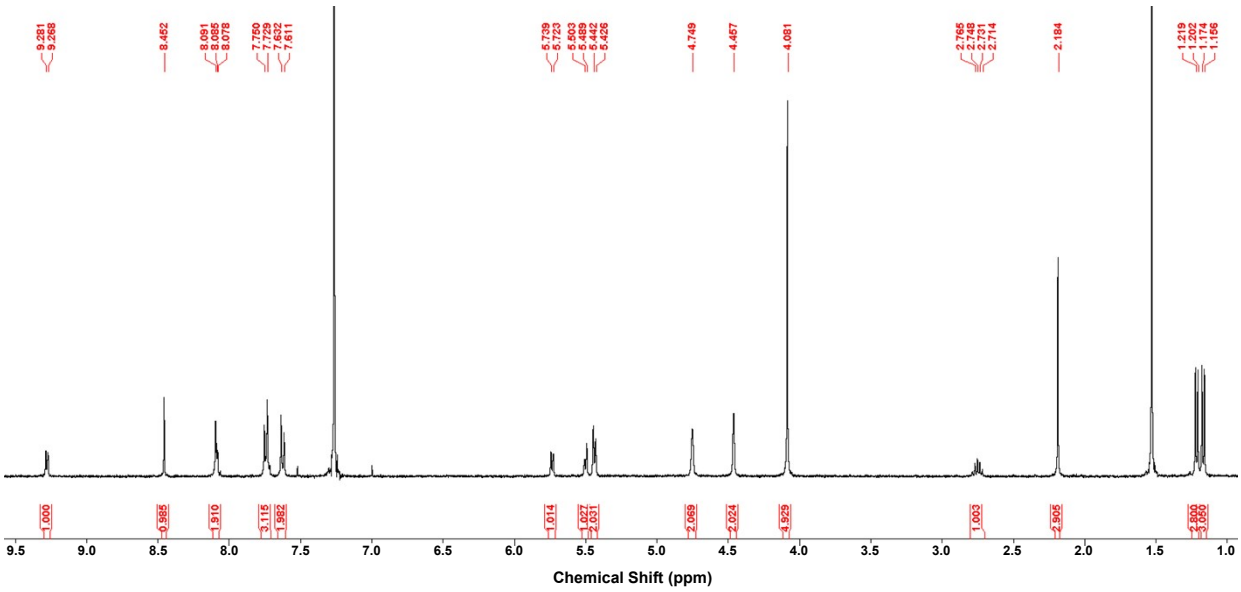

Figure S2. ^{1}H NMR of **C2** in $CDCl_3$.

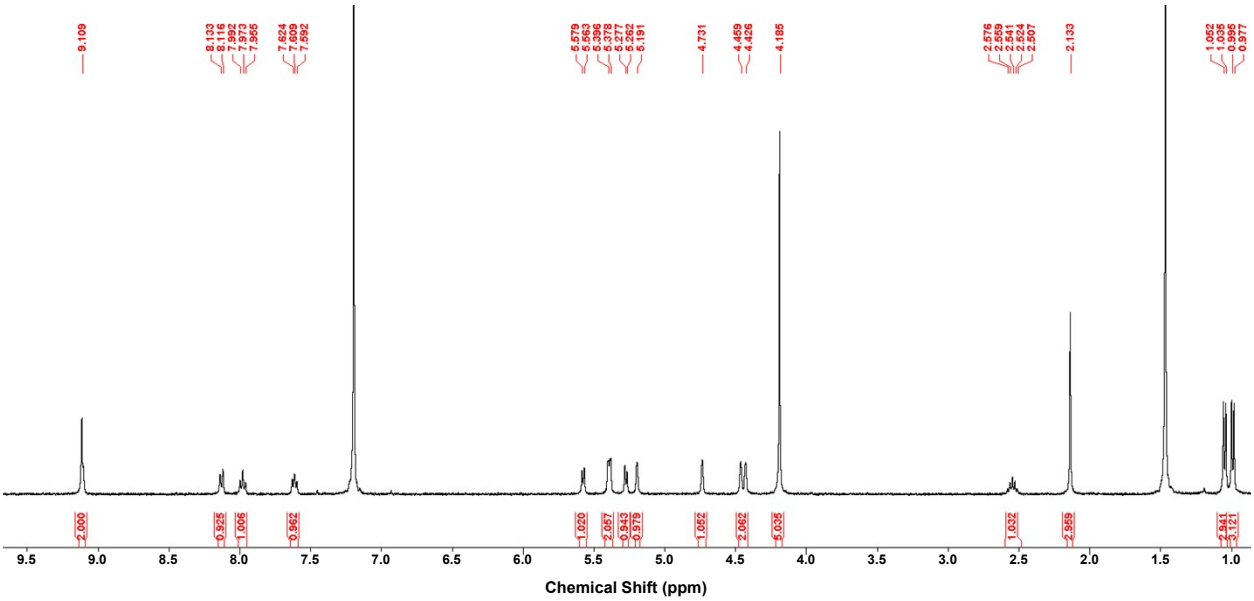

Figure S3. ^{1}H NMR of **C3** in $CDCl_3$.

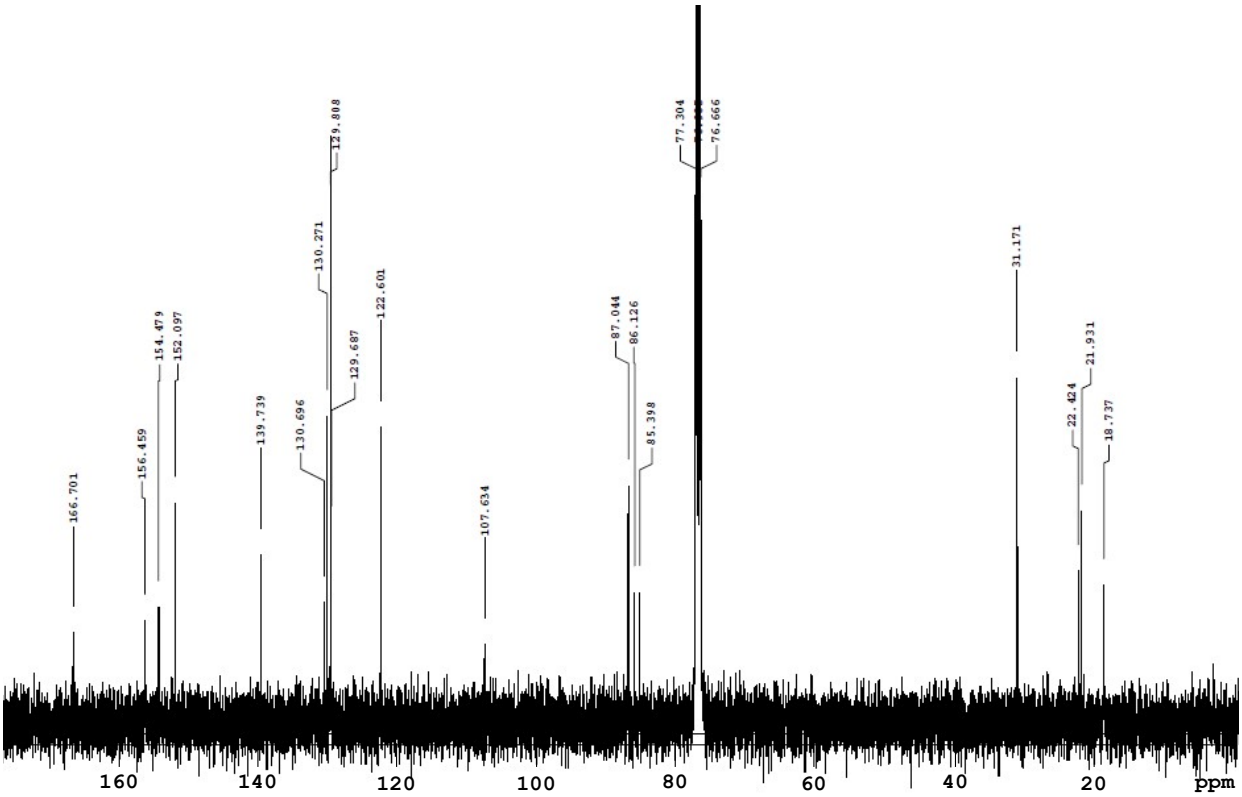

Figure S4. ^{13}C NMR of **C1** in $CDCl_3$.

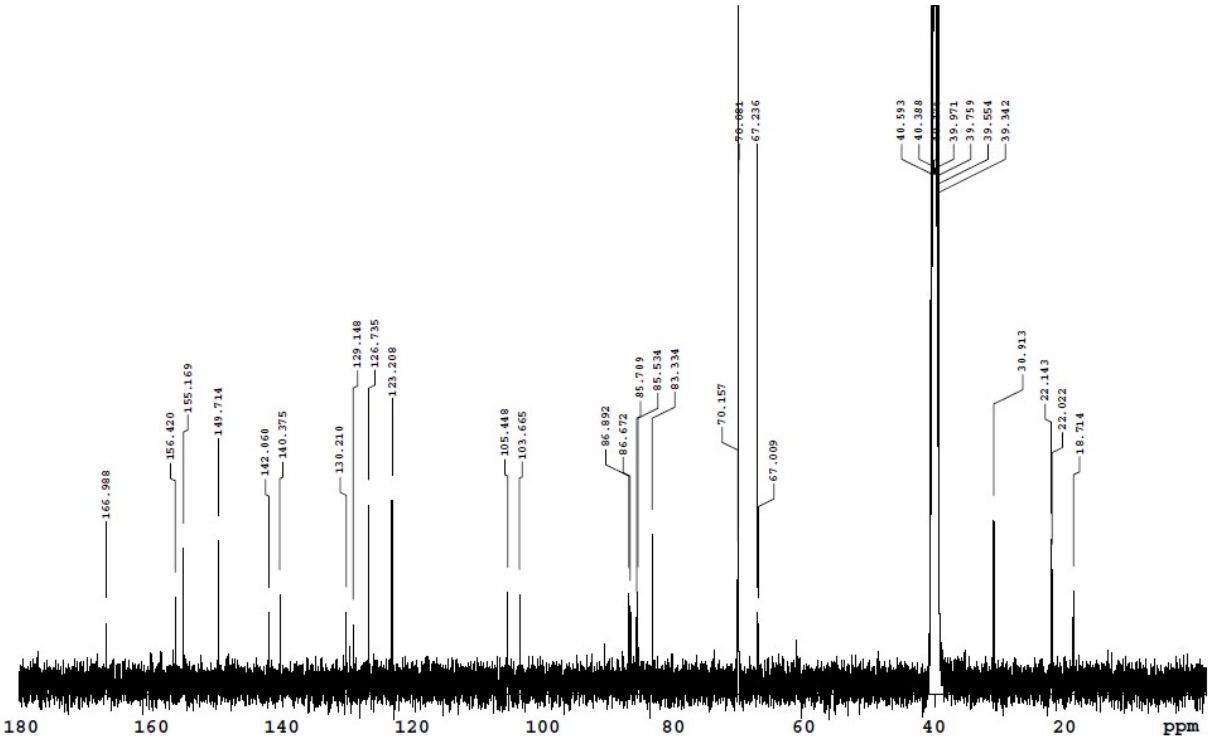

Figure S5. ^{13}C NMR of **C2** in D_6-DMSO.

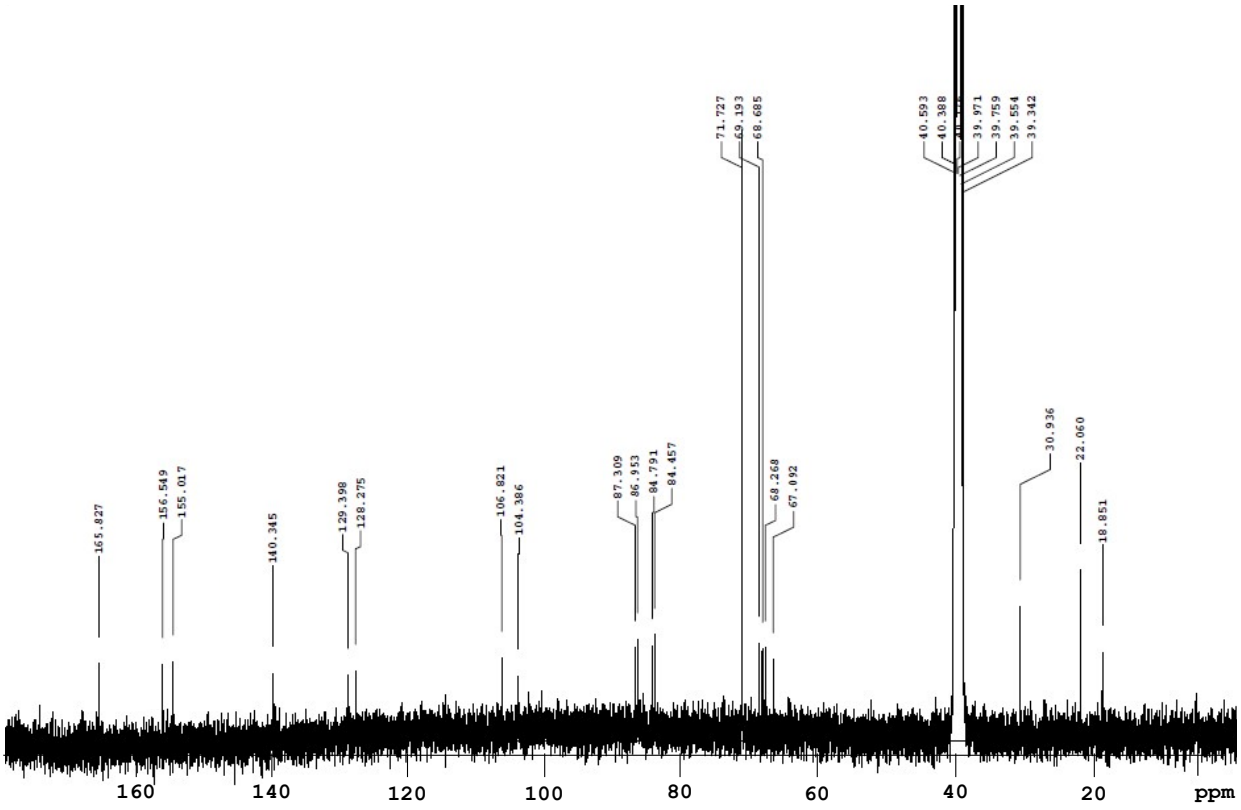

Figure S6. ^{13}C NMR of **C3** in D_6-DMSO.

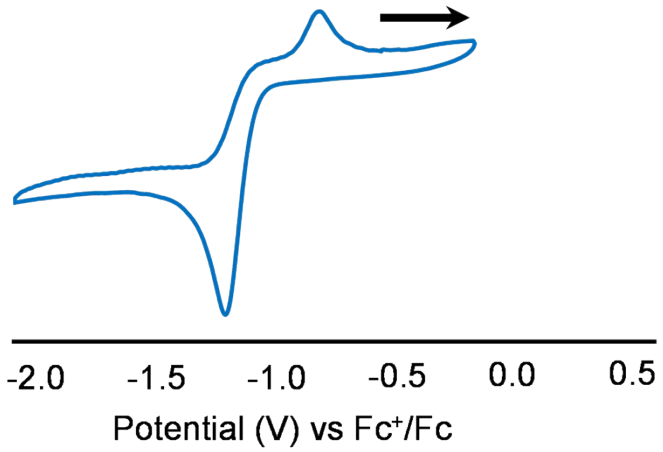

Figure S7. Cyclic voltammogram of **C1** (1 mM) in CH_2Cl_2 containing 0.1 M $[NBu_4][PF_6]$, where the scan direction is indicated by the arrow. An irreversible redox couple was observed with reduction potentials of −0.80 V and −1.23 V.

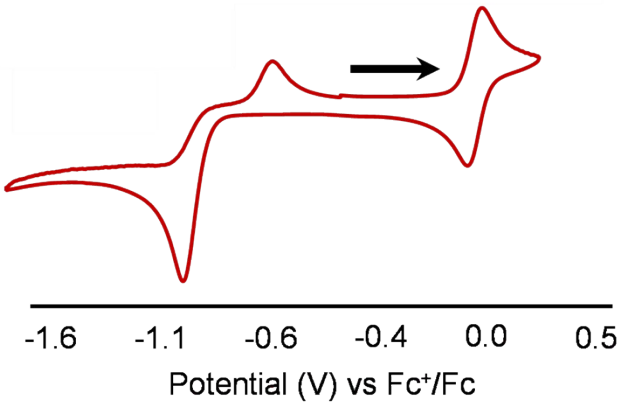

Figure S8. Cyclic voltammogram of **C2** (1 mM) in CH_2Cl_2 containing 0.1 M $[NBu_4][PF_6]$, where the scan direction is indicated by the arrow.

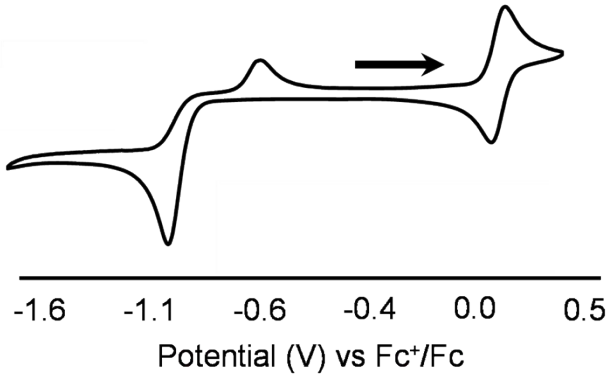

Figure S9. Cyclic voltammogram of **C3** (1 mM) in CH_2Cl_2 containing 0.1 M $[NBu_4][PF_6]$, where the scan direction is indicated by the arrow.

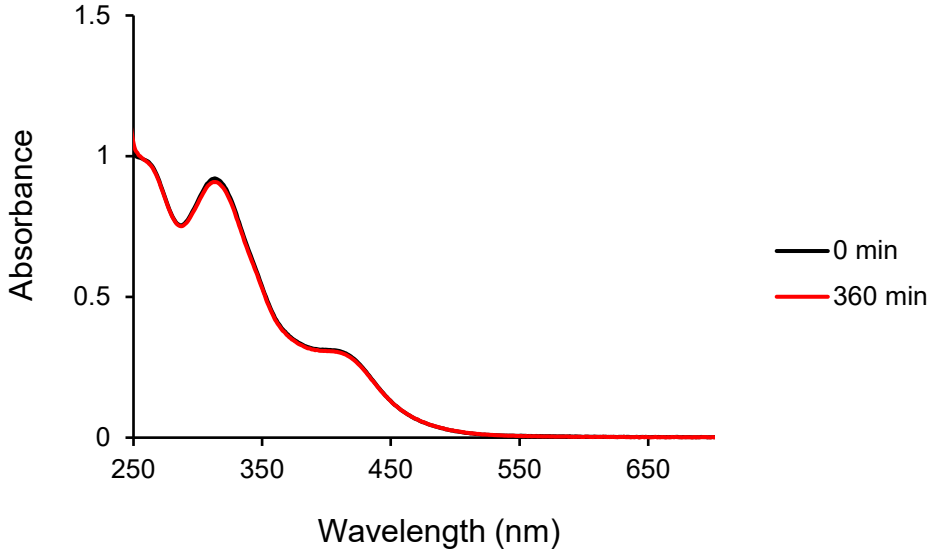

Figure S10. UV-Vis spectra of complex **C1** (100 μM) incubated in PBS (pH 7.4) at 37 °C for 6 hours.

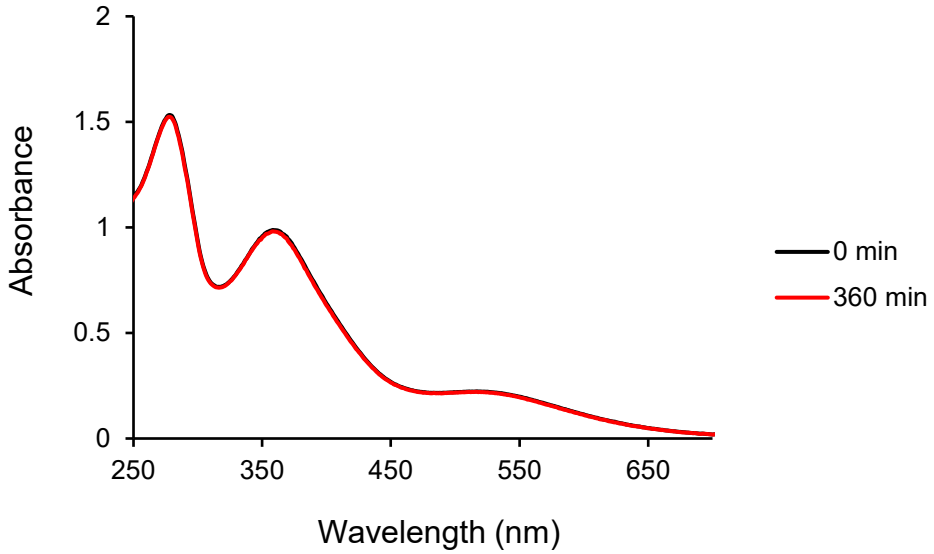

Figure S11. UV-Vis spectra of complex **C2** (100 μM) incubated in PBS (pH 7.4) at 37 °C for 6 hours.

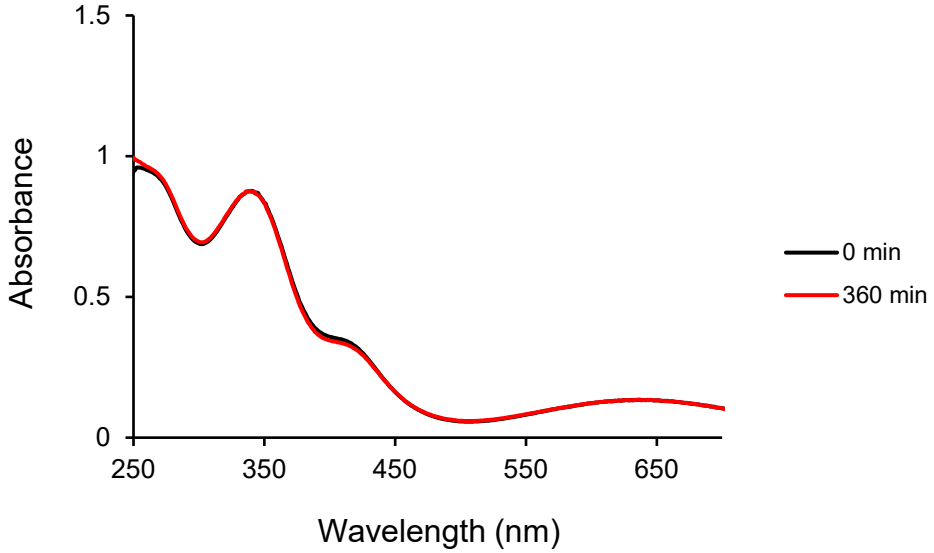

Figure S12. UV-Vis spectra of complex **C3** (100 μM) incubated in PBS (pH 7.4) at 37 °C for 6 hours.

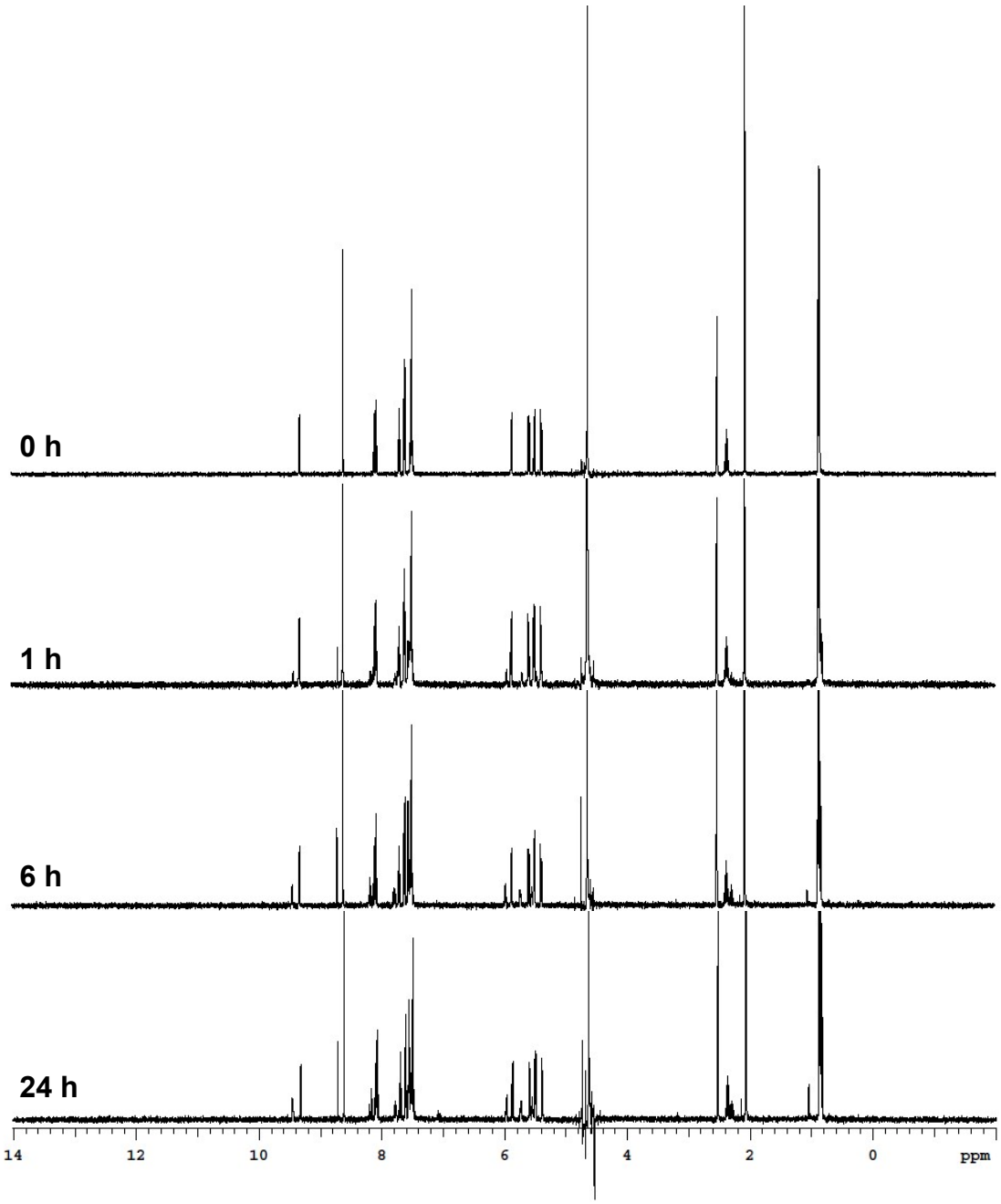

Figure S13. ^{1}H NMR of **C1** in D_2O and 10% D_6-DMSO over prolonged periods of incubation at 37°C.

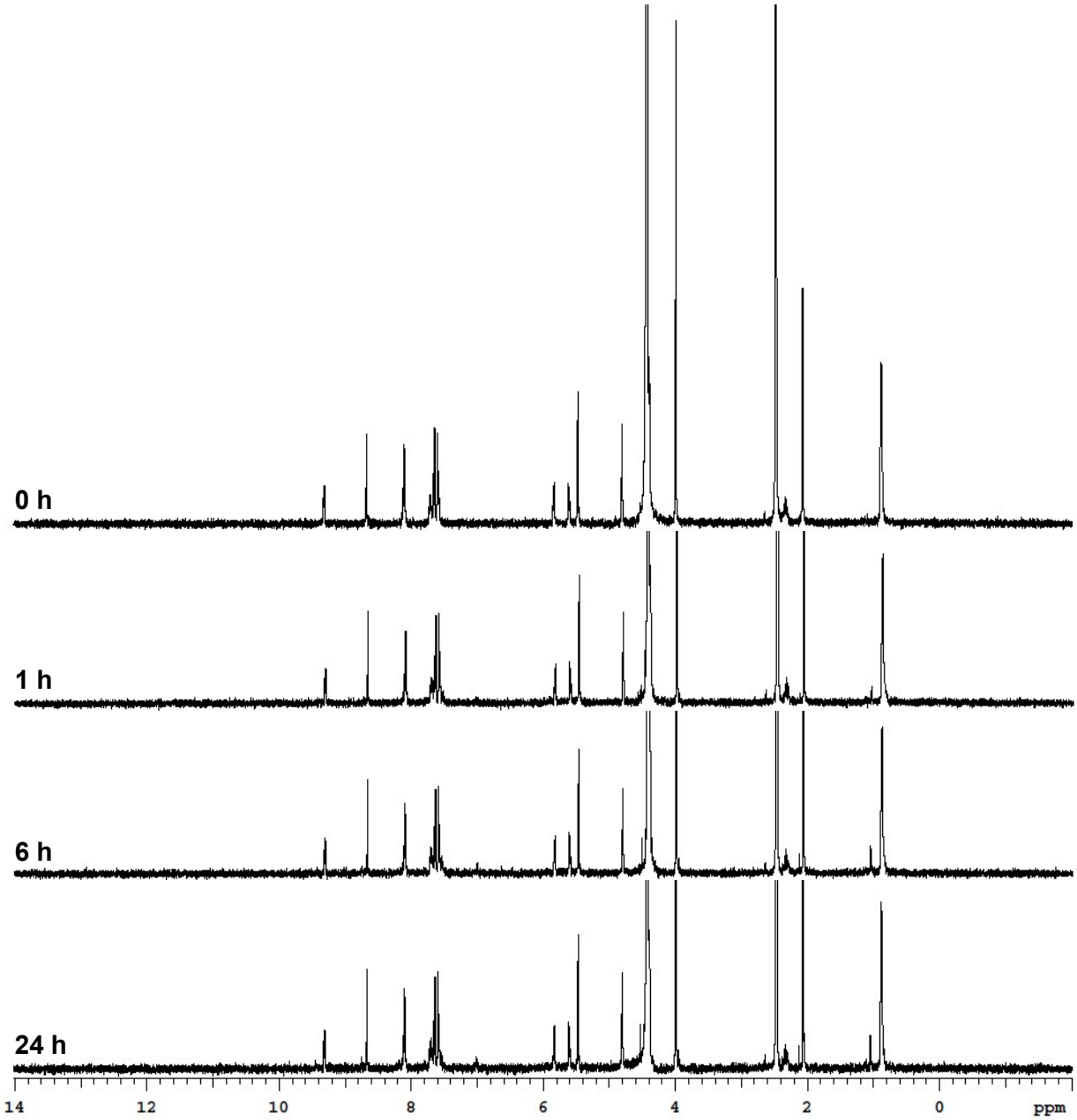

Figure S14. ^{1}H NMR of **C2** in D_2O and 50% D_6-DMSO over prolonged periods of incubation at 37°C.

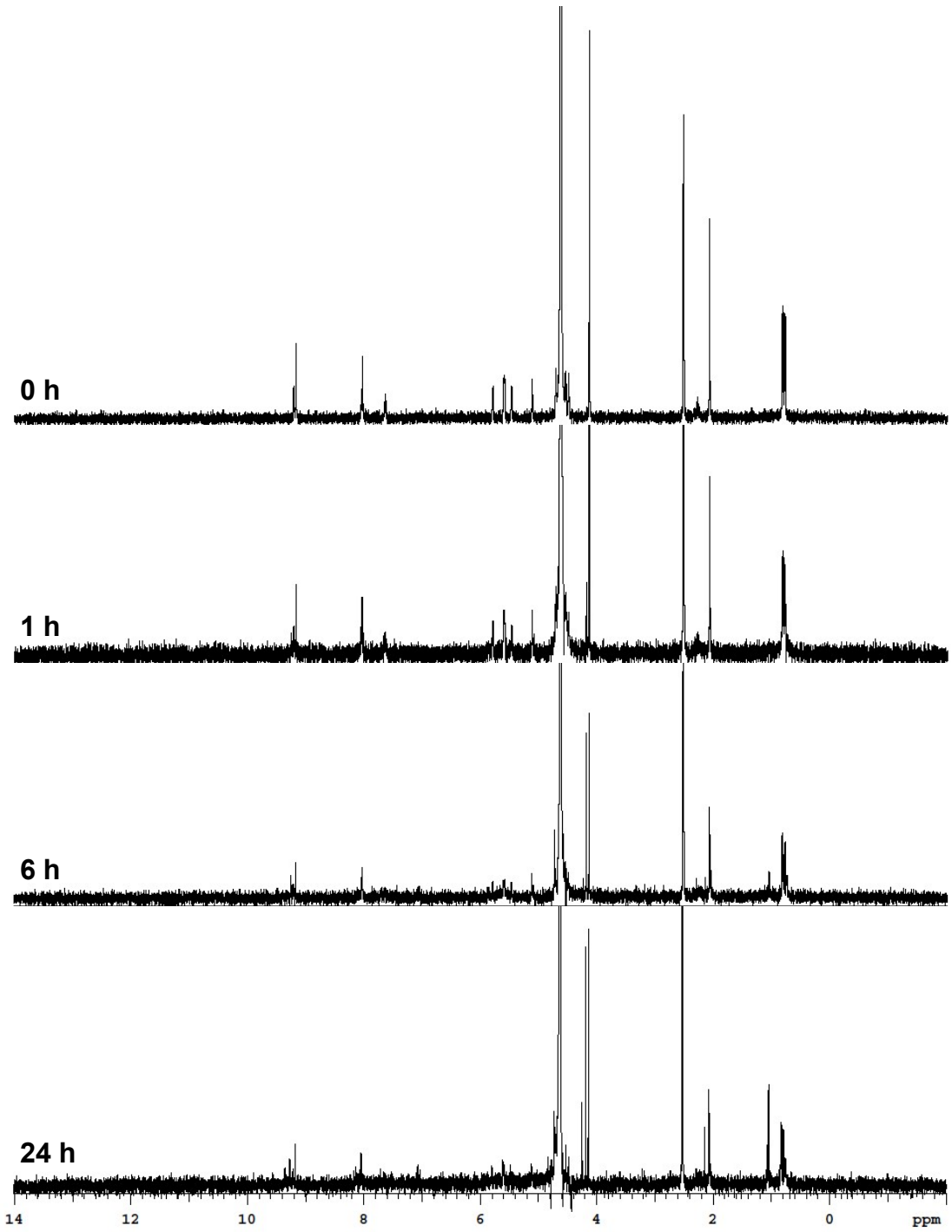

Figure S15. ^{1}H NMR of **C3** in D_2O and 10% D_6-DMSO over prolonged periods of incubation at 37°C.

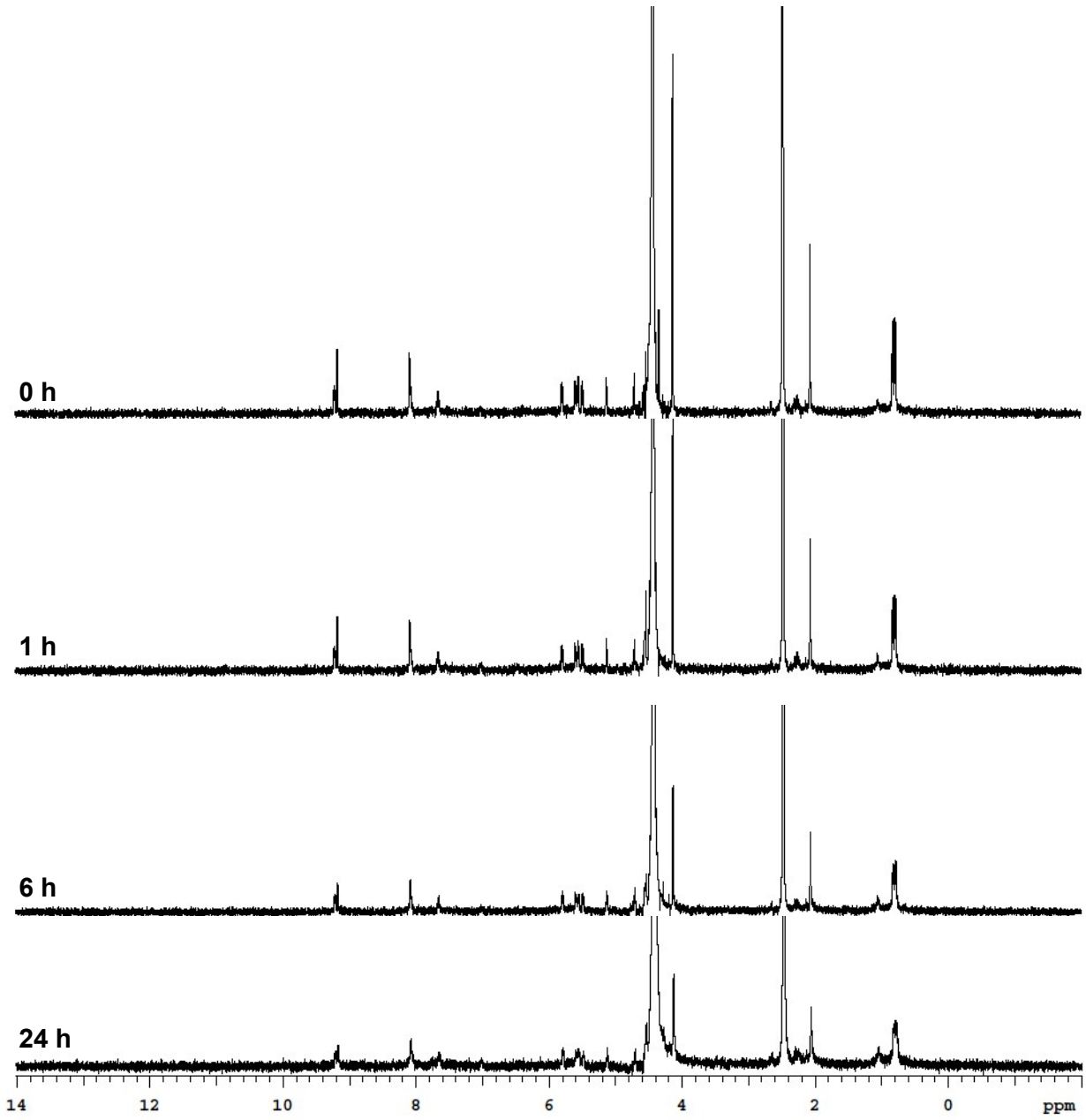

Figure S16. ^{1}H NMR of **C3** in D_2O and 50% D_6-DMSO over prolonged periods of incubation at 37°C.

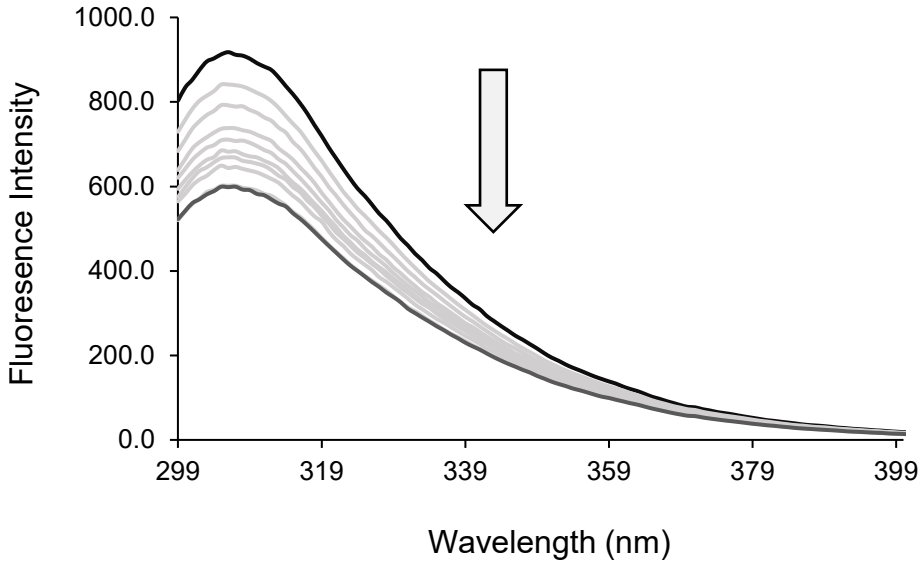

Figure S17. Fluorescence emission spectra at various complex-to-HSA ratios by the titration of HSA with **C1** using λ_{ex} = 260 nm where the [HSA] = 10 μM and the [Ru] = 0-25 μM.

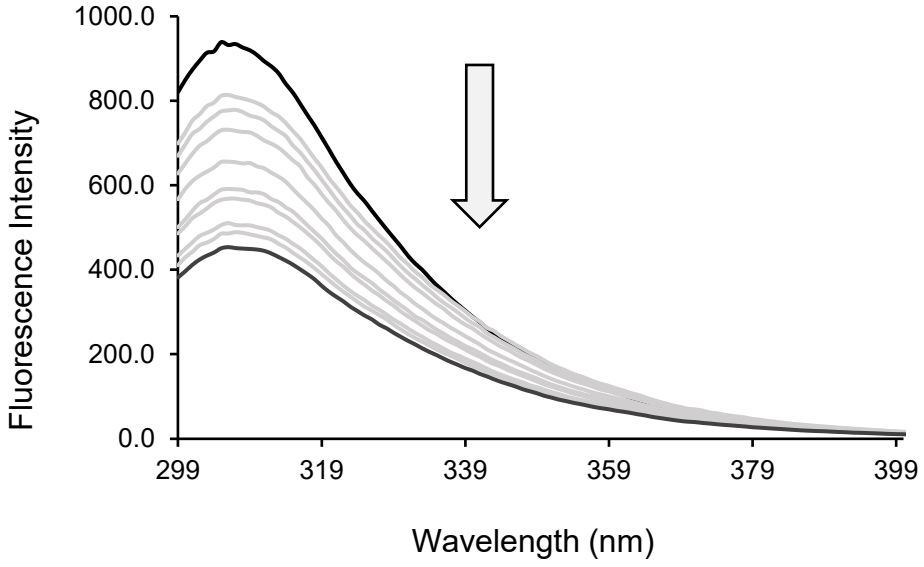

Figure S18. Fluorescence emission spectra at various complex-to-HSA ratios by the titration of HSA with **C2** using λ_{ex} = 260 nm where the [HSA] = 10 μM and the [Ru] = 0-25 μM.

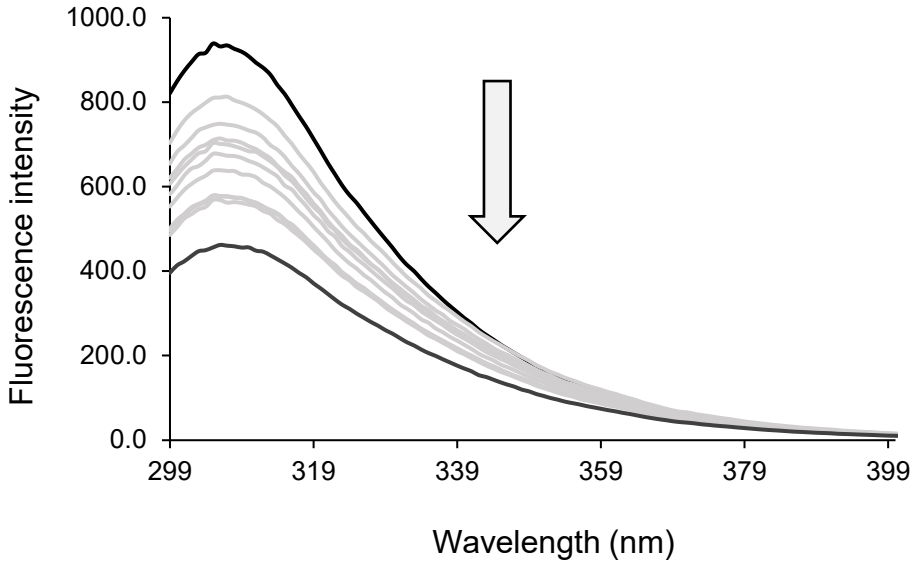

Figure S19. Fluorescence emission spectra at various complex-to-HSA ratios by the titration of HSA with **C3** using λ_{ex} = 260 nm where the [HSA] = 10 μM and the [Ru] = 0-25 μM.

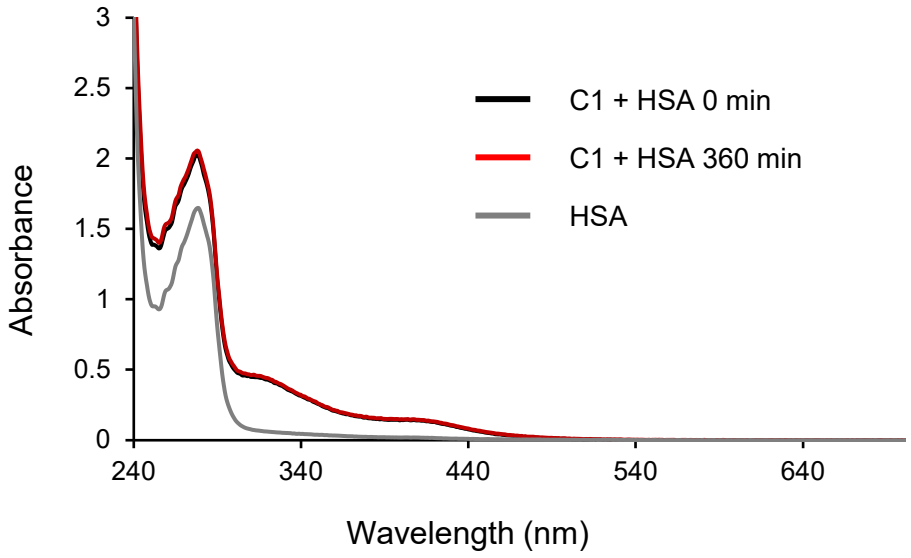

Figure S20. UV-Vis spectra of complex **C1** (50 μM) incubated with HSA (50 μM) in PBS buffer (pH 7.4) for 6 hours at 37 °C.

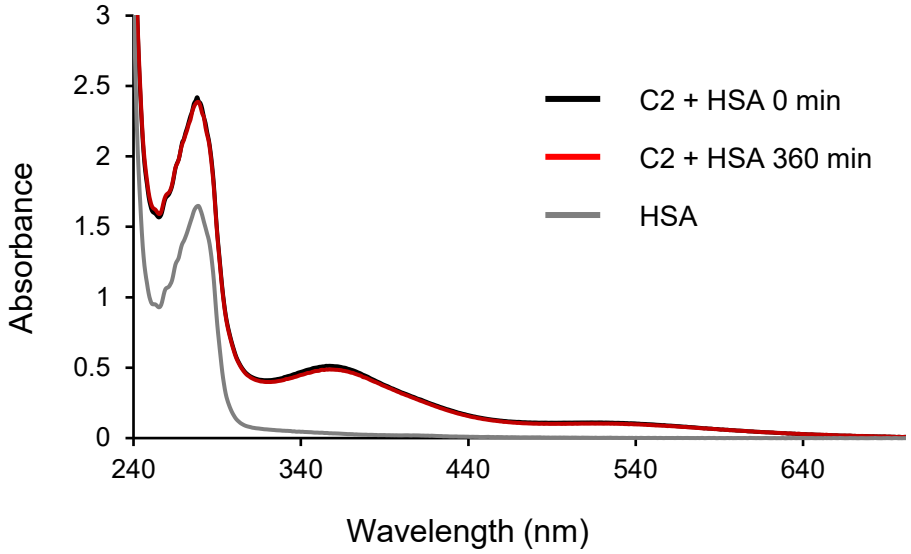

Figure S21. UV-Vis spectra of complex **C2** (50 μM) incubated with HSA (50 μM) in PBS buffer (pH 7.4) for 6 hours at 37 °C.

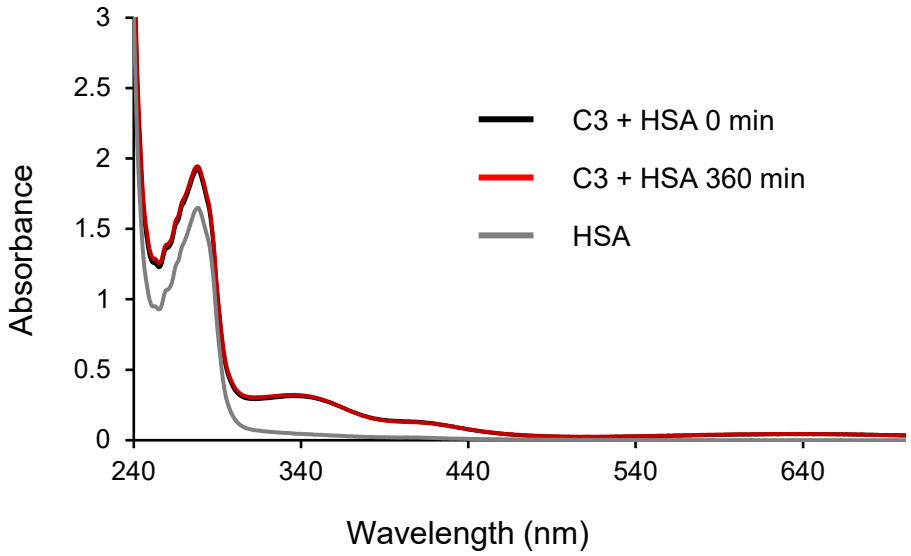

Figure S22. UV-Vis spectra of complex **C3** (50 μM) incubated with HSA (50 μM) in PBS buffer (pH 7.4) for 6 hours at 37 °C.

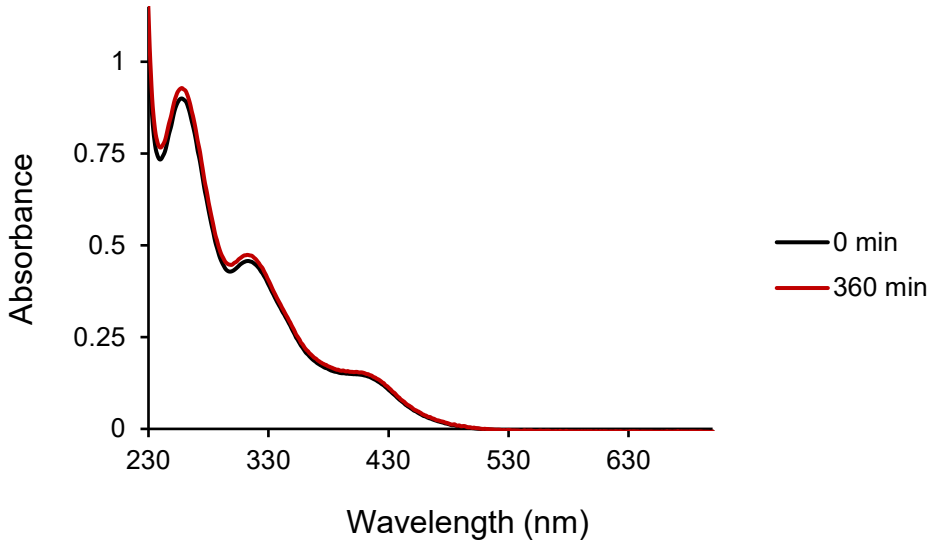

Figure S23. UV-Vis spectra of complex **C1** (50 μM) incubated with CT-DNA (50 μM) in Tris-HCl buffer (pH 7.0) for 6 hours at 37 °C.

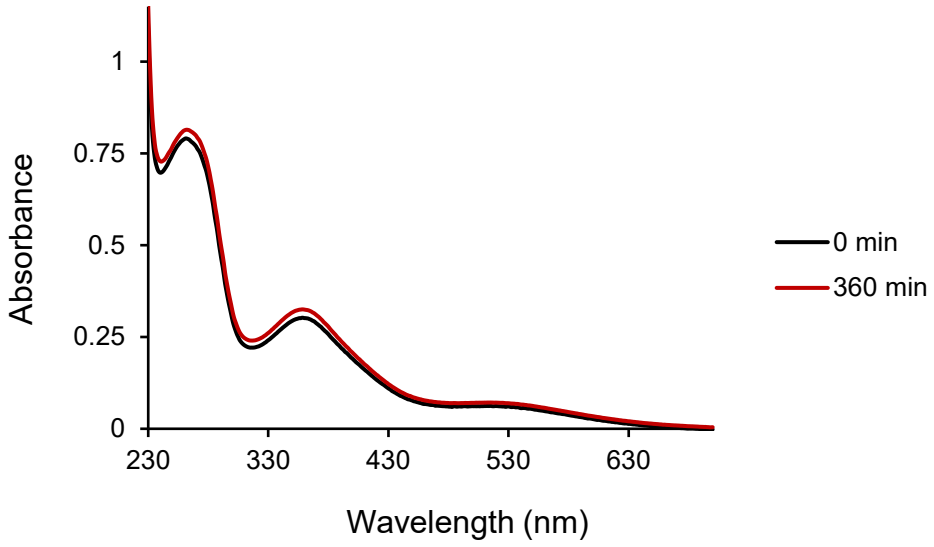

Figure S24. UV-Vis spectra of complex **C2** (50 μM) incubated with CT-DNA (50 μM) in Tris-HCl buffer (pH 7.0) for 6 hours at 37 °C.

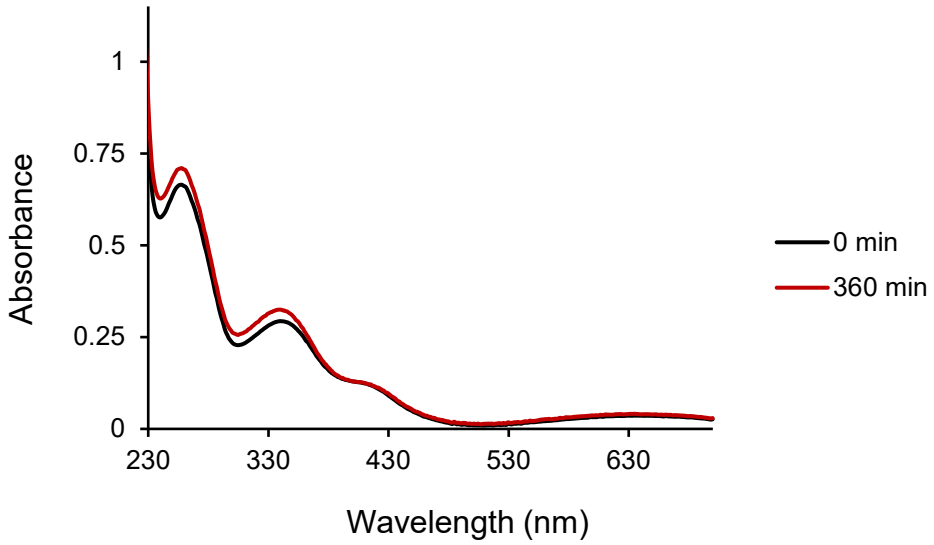

Figure S25. UV-Vis spectra of complex **C3** (50 μM) incubated with CT-DNA (50 μM) in Tris-HCl buffer (pH 7.0) for 6 hours at 37 °C.

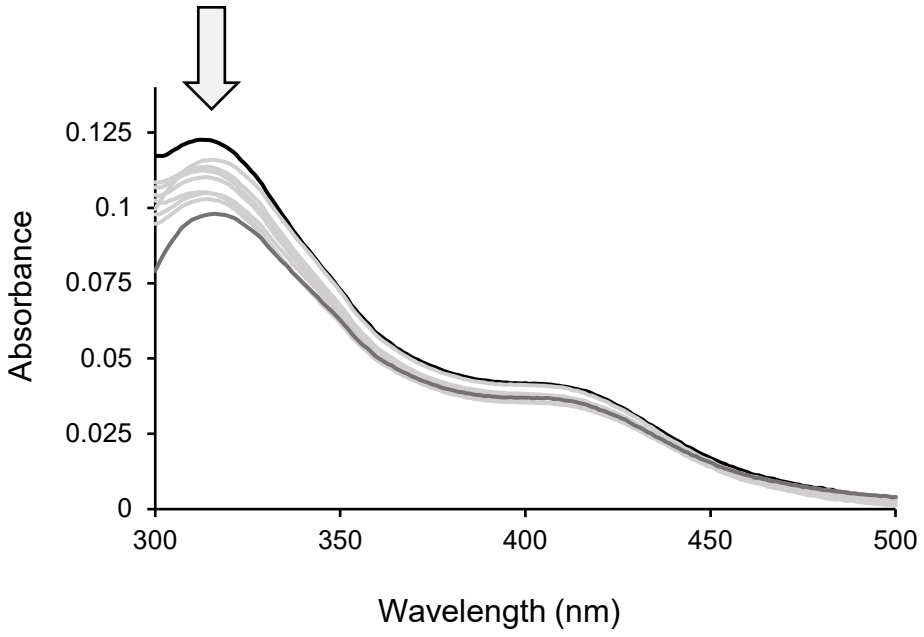

Figure S26. UV-Vis spectra of complex **C1** (30 μM) with CT-DNA (0 - 90 μM) in Tris-HCl buffer (pH 7.0) after 1 hour of incubation at 37 °C.

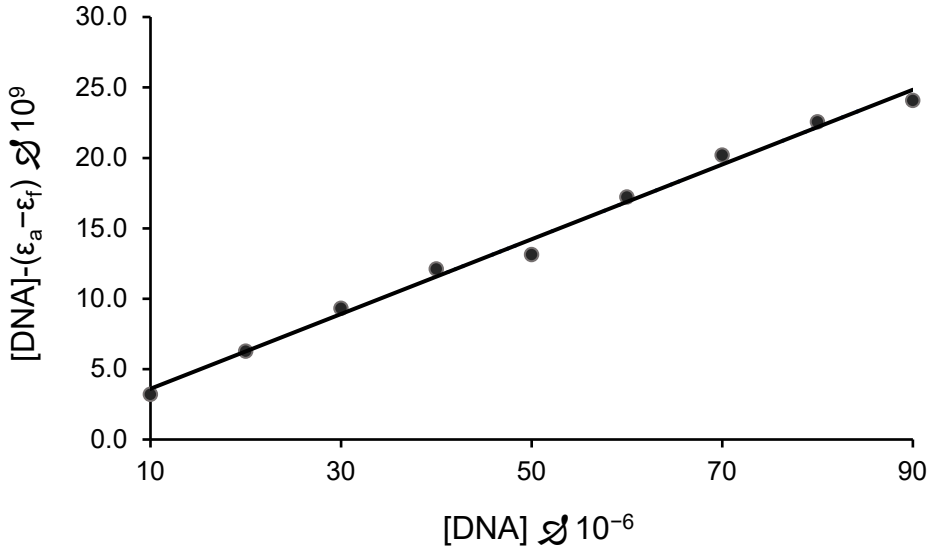

Figure S27. Plot of [DNA] / ($\varepsilon_A - \varepsilon_F$) versus [DNA] for the titration of **C1** with CT-DNA.

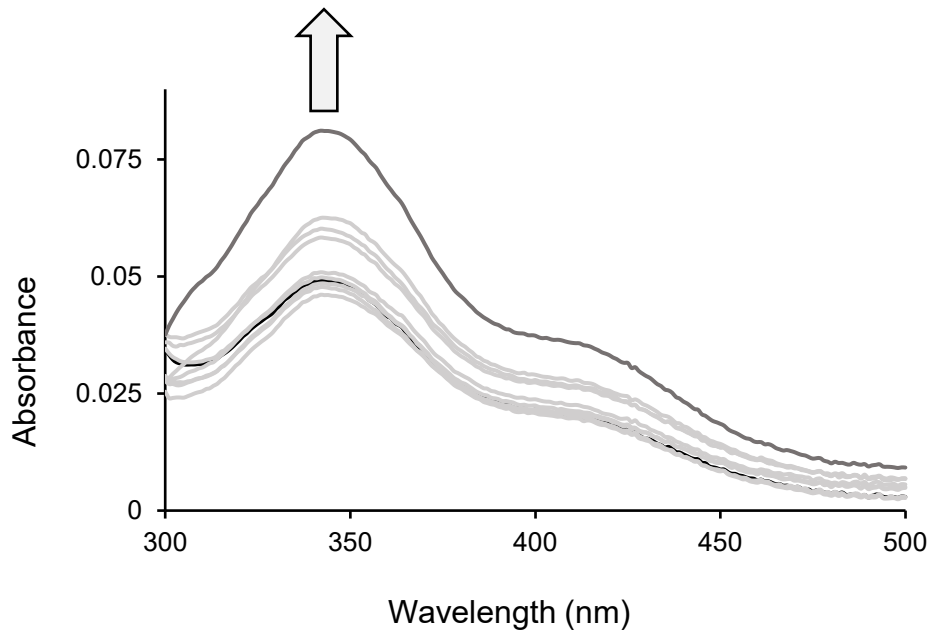

Figure S28. UV-Vis spectra of complex **C3** (30 μM) with CT-DNA (0 - 90 μM) in Tris-HCl buffer (pH 7.0) after 1 hour of incubation at 37 °C.

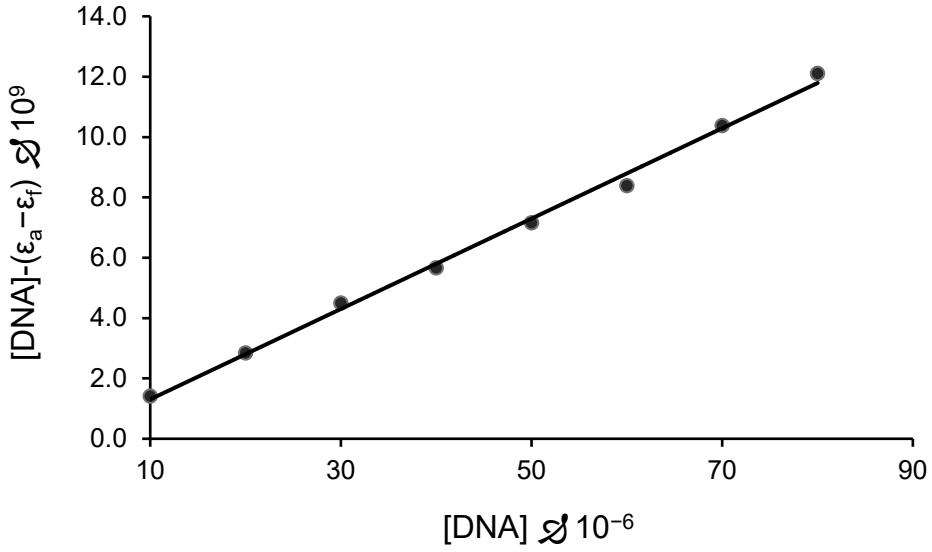

Figure S29. Plot of [DNA] / ($\varepsilon_A - \varepsilon_F$) versus [DNA] for the titration of **C3** with CT-DNA.

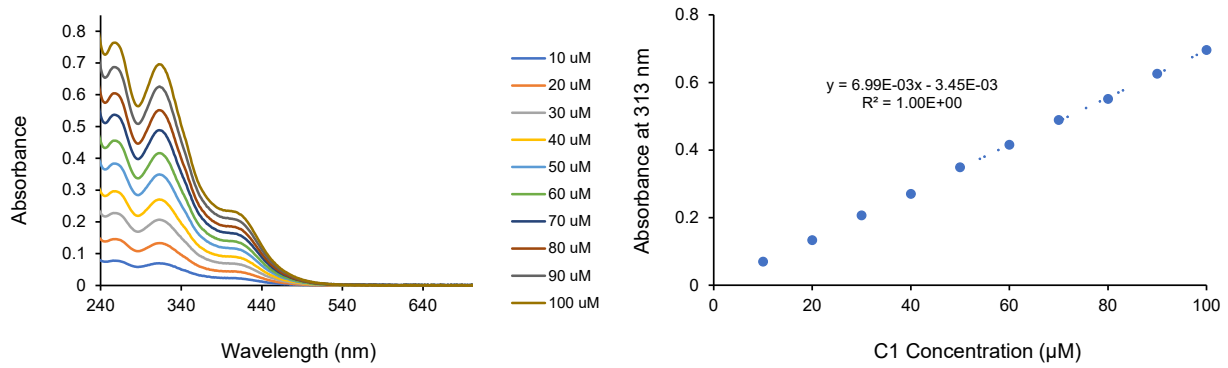

Figure S30. Calibration curve of **C1** in PBS (pH 7.4) to determine the extinction coefficient.

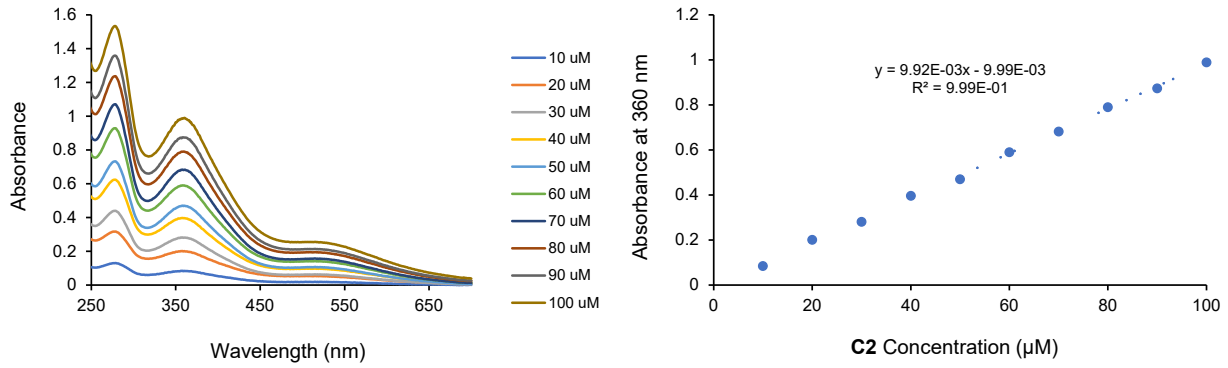

Figure S31. Calibration curve of **C2** in PBS (pH 7.4) to determine the extinction coefficient.

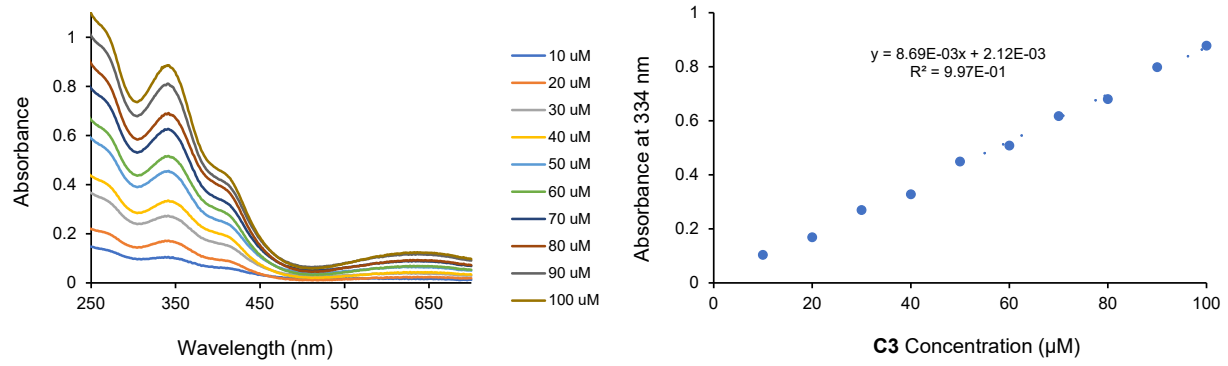

Figure S32. Calibration curve of **C3** in PBS (pH 7.4) to determine the extinction coefficient.

Table S1. Crystallographic data for complexes **C1** and **C3**.

	C1	**C3**
CCDC Number	2192092	2013493
molecular formula	$C_{22}H_{24}ClF_6N_2PRu \cdot C_3H_6O$	$C_{26}H_{28}ClF_6FeN_2PRu$
fw	656.00	705.84
crystal size (mm)	0.36 × 0.12 × 0.05	0.37 × 0.34 × 0.32
temp (K)	100(2)	100(2)
Crystal system	Triclinic	Monoclinic
space group	P1bar	$P2_1/c$
a (Å)	9.1814(8)	18.600(2)
b (Å)	12.3291(11)	20.872(2)
c (Å)	12.6542(12)	13.7091(12)
α (°)	76.919(5)	90
β (°)	73.108(5)	88.123(7)
γ (°)	87.998(5)	90
V (Å^3)	1334.3(2)	5319.3(10)
Z	2	8
Wavelength (Å)	0.71073	0.71073
ρ_{calcd} (g/cm^3)	1.633	1.763
μ (mm^{-1})	0.812	1.336
θ range	1.70 – 27.73	1.10 – 32.12
refl. collected	43026	18735
indep. refl. / R_{int}	6226 / 0.030	18735 / 0.031
data/restraints/ parameters	43026 / 6226 / 0	18735 / 804 / 295
R indices [I>2σ(I)]; R_1/wR_2	0.0199 / 0.0466	0.0306 / 0.0773
R indices all data; R_1/wR_2	0.0234 / 0.0482	0.0417 / 0.0844
largest peak/hole (eÅ^{-3})	0.703 / −0.409	0.977 / −0.678
GOF	1.035	1.079