

Supporting Information

**DNA interaction of ruthenium(II) complexes with imidazo[4,5-
f][1,10]phenanthroline derivatives**

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- Fig. S9.** Changes in the absorption spectra of complex **4** (10 μM) under visible irradiation in the presence of CT-DNA (1 mM) at pH 7.0. a) Air-saturated solution, b) Argon-saturated solution. Irradiation: t = 0, 0.5, 1, 2, 3 h.

Table S1 Crystal data and structure refinement for complex **2**.

Empirical formula	C ₄₃ H ₃₀ Cl ₂ N ₈ O ₈ Ru
Formula weight	958.72
Crystal system	orthorhombic
Space group	Pnma
Unit cell dimensions	a = 26.3477(2) Å b = 20.8970(2) Å c = 18.0176(2) Å α = 90° β = 90° γ = 90°
Volume	9920.27(16) Å ³
Z	8
Calculated density	1.284 g/cm ³
Absorption coefficient	4.006 mm ⁻¹
F(000)	3888.0
Crystal size	0.47 × 0.42 × 0.25 mm ³
Radiation	Cu Kα (λ = 1.54178)
θ range for data collection/°	6.71 – 125.224
Index ranges	-29 ≤ h ≤ 22 -22 ≤ k ≤ 23 -19 ≤ l ≤ 20
Reflections collected	21833
Independent reflections	7939 [R _{int} = 0.0315, R _{sigma} = 0.0554]
Data/restraints/parameters	7939 / 72 / 577
Goodness-of-fit on F ²	0.967
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0467, wR ₂ = 0.1231
Final R indexes [all data]	R ₁ = 0.0666, wR ₂ = 0.1297
Largest diff. peak/hole / e Å ⁻³	0.92 and -0.90

Table S2 Selected bond lengths (Å) and angles(°) for complex **2**.

Ru1 - N1	2.057(4)	Ru1 - N2	2.057(4)
Ru1 - N5	2.061(4)	Ru1 - N6	2.050(4)
Ru1 - N7	2.053(4)	Ru1 - N8	2.053(4)
N1 - Ru1 - N2	79.59(14)	N1 - Ru1 - N5	98.02(14)
N1 - Ru1 - N6	89.10(14)	N1 - Ru1 - N7	96.01(14)
N1 - Ru1 - N8	173.39(14)	N2 - Ru1 - N5	173.53(15)
N2 - Ru1 - N6	94.43(16)	N2 - Ru1 - N7	90.75(14)
N2 - Ru1 - N8	96.17(14)	N5 - Ru1 - N6	79.47(16)
N5 - Ru1 - N7	95.50(15)	N5 - Ru1 - N8	86.72(14)
N7 - Ru1 - N8	78.89(14)		

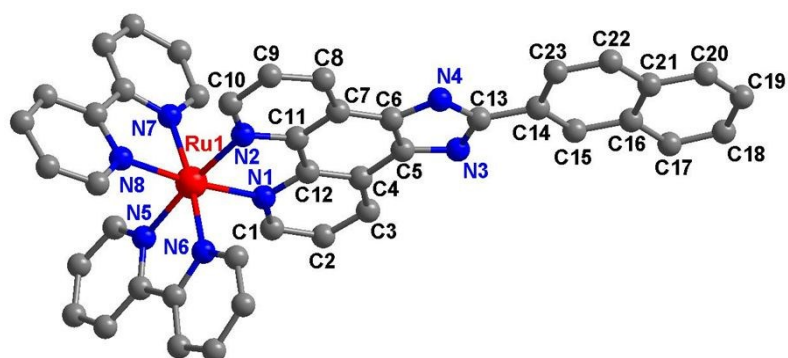


Fig. S1. X-ray crystal structure of complex **2**. The H atoms, counter anion and solvent have been omitted for clarity. Only the major conformation of the disorder is shown in this figure.

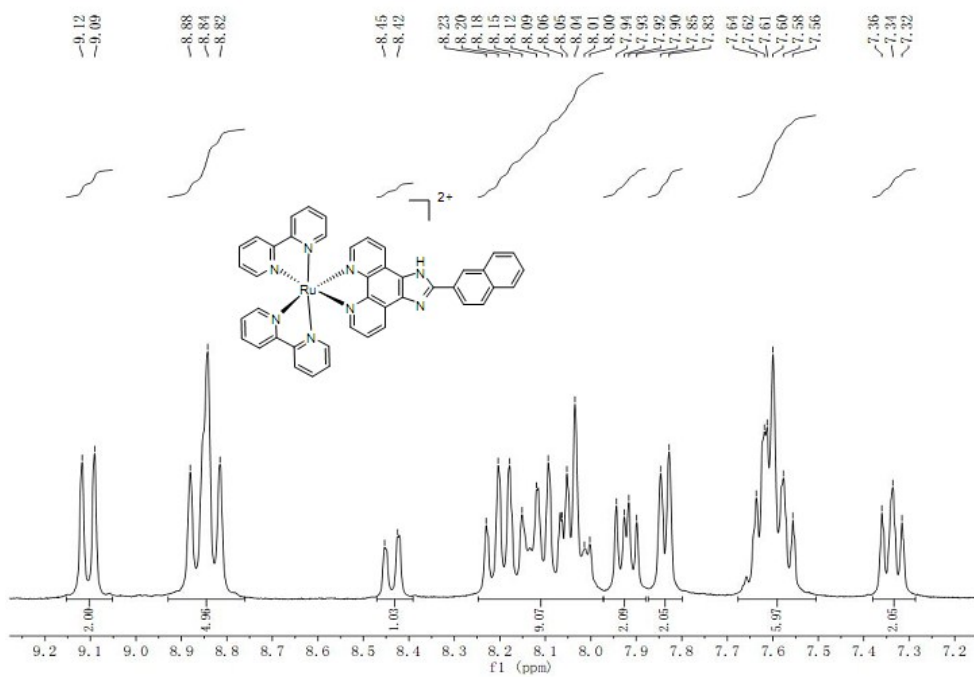


Fig. S2. ¹H NMR spectrum of complex 2.

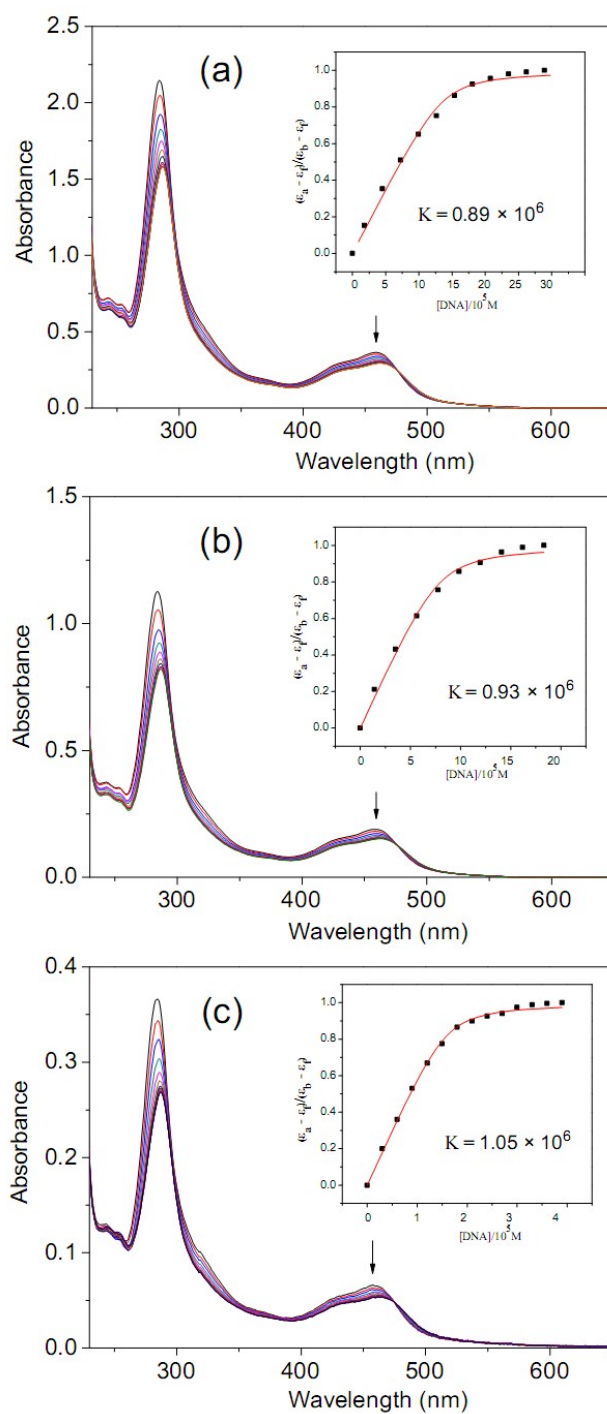


Fig. S3. Absorption spectra of complex **1** at 20 μM (a), 10 μM (b) and 4 μM (c) upon addition of CT-DNA. Arrows indicate the change in absorbance upon increasing the DNA concentration. Insert: Plot of $(\epsilon_a - \epsilon_f)/(\epsilon_b - \epsilon_f)$ vs $[\text{DNA}]$ for the titration of DNA to complex **1**.

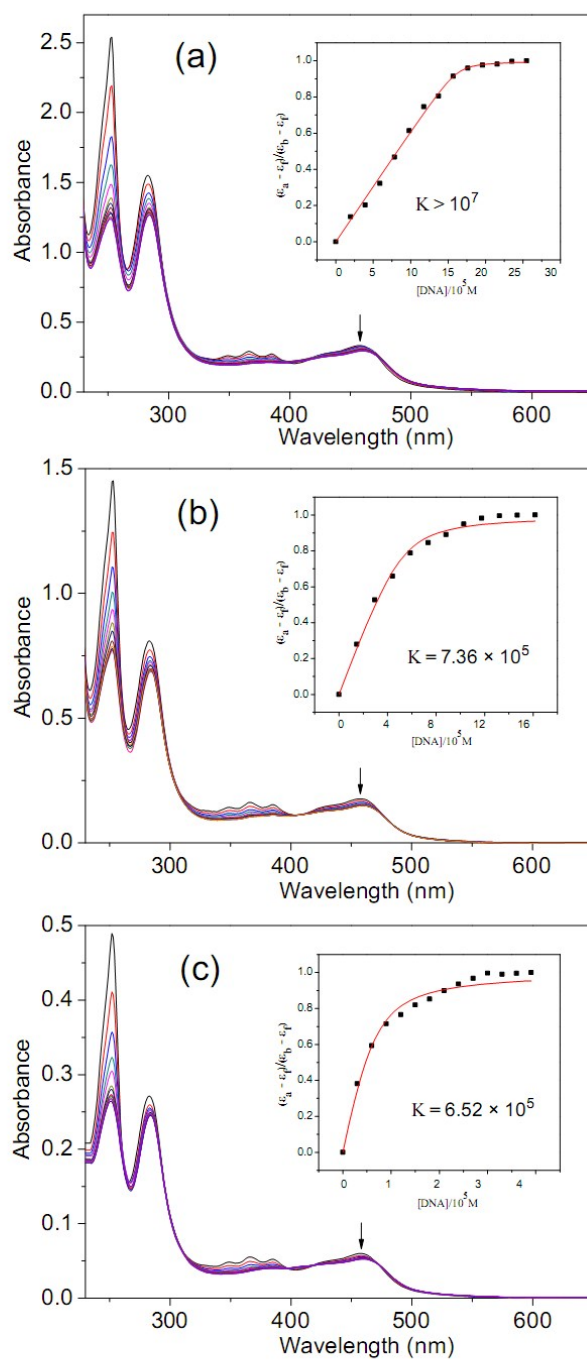


Fig. S4. Absorption spectra of complex **3** at 20 μM (a), 10 μM (b) and 4 μM (c) upon addition of CT-DNA. Arrows indicate the change in absorbance upon increasing the DNA concentration. Insert: Plot of $(\epsilon_a - \epsilon_f)/(\epsilon_b - \epsilon_f)$ vs $[DNA]$ for the titration of DNA to complex **3**.

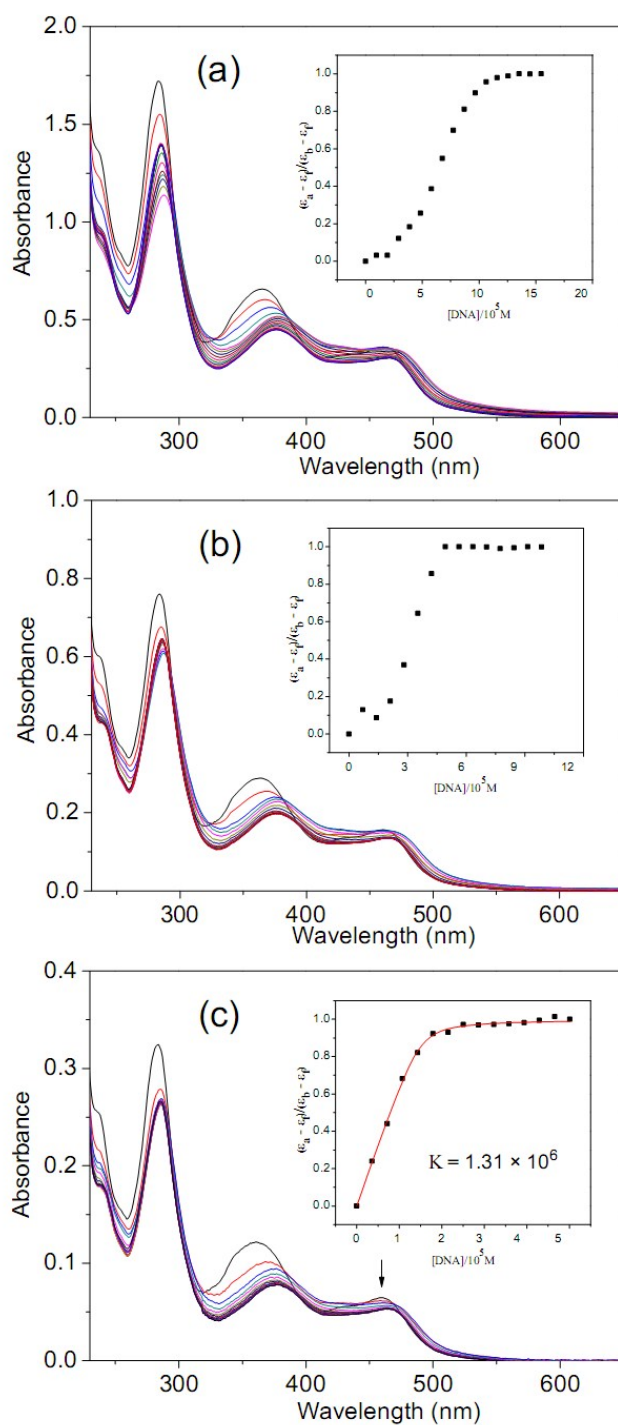


Fig. S5. Absorption spectra of complex 4 at 20 μM (a), 10 μM (b) and 4 μM (c) upon addition of CT-DNA. Arrows indicate the change in absorbance upon increasing the DNA concentration. Insert: Plot of $(\epsilon_a - \epsilon_f)/(\epsilon_b - \epsilon_f)$ vs $[DNA]$ for the titration of DNA to complex 4.

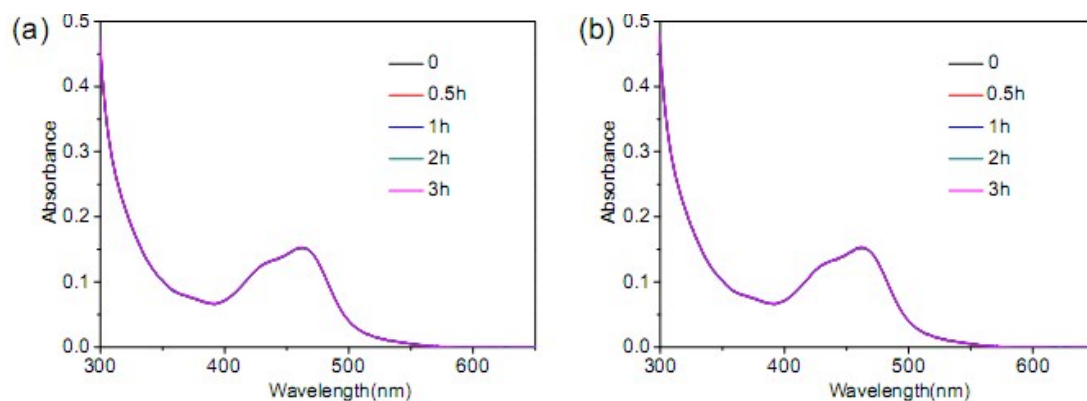


Fig. S6. Changes in the absorption spectra of complex **1** ($10 \mu\text{M}$) under visible irradiation in the presence of CT-DNA (1 mM) at pH 7.0. a) Air-saturated solution, b) Argon-saturated solution. Irradiation: $t = 0, 0.5, 1, 2, 3 \text{ h}$.

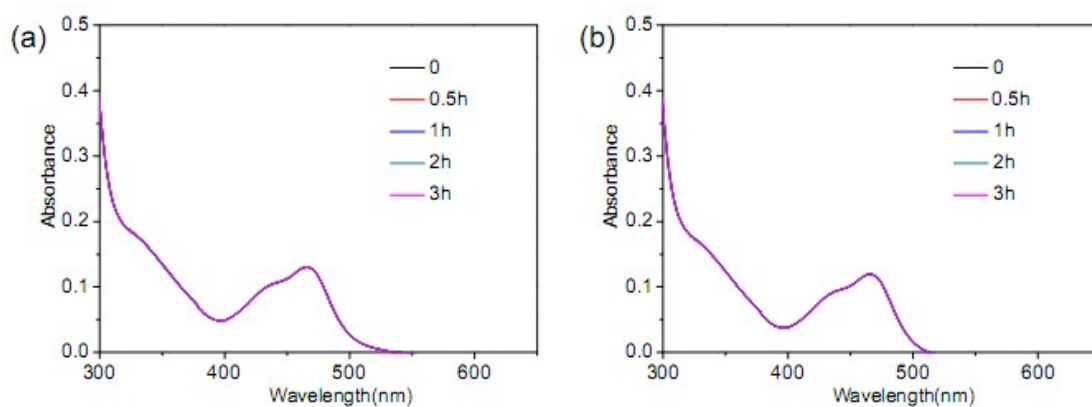


Fig. S7. Changes in the absorption spectra of complex **2** ($10 \mu\text{M}$) under visible irradiation in the presence of CT-DNA (1 mM) at pH 7.0. a) Air-saturated solution, b) Argon-saturated solution. Irradiation: $t = 0, 0.5, 1, 2, 3 \text{ h}$.

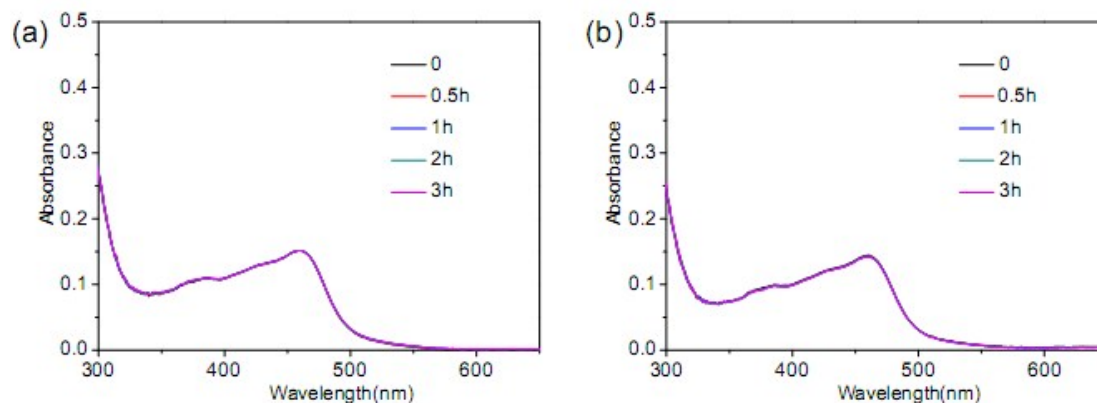


Fig. S8. Changes in the absorption spectra of complex 3 ($10 \mu\text{M}$) under visible irradiation in the presence of CT-DNA (1 mM) at pH 7.0. a) Air-saturated solution, b) Argon-saturated solution. Irradiation: $t = 0, 0.5, 1, 2, 3$ h.

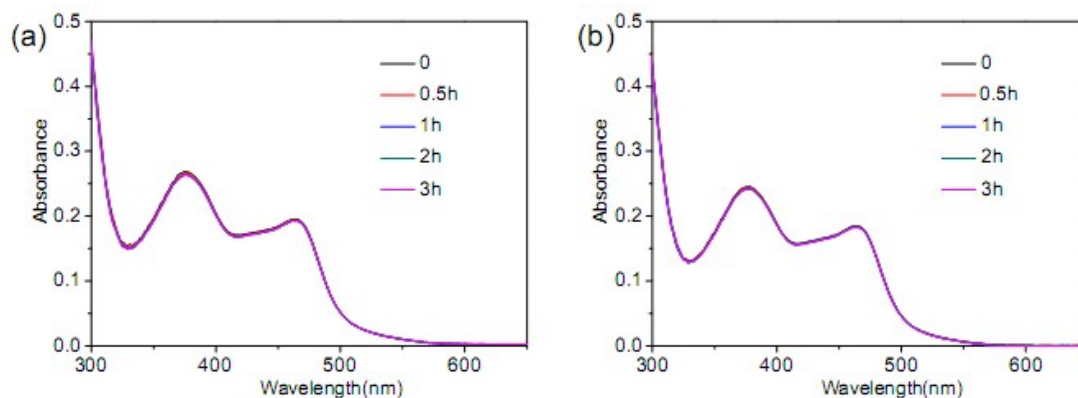


Fig. S9. Changes in the absorption spectra of complex 4 ($10 \mu\text{M}$) under visible irradiation in the presence of CT-DNA (1 mM) at pH 7.0. a) Air-saturated solution, b) Argon-saturated solution. Irradiation: $t = 0, 0.5, 1, 2, 3$ h.