Supplementary Information

DNA-interacting properties of two analogous square-planar *cis*-chlorido complexes: copper *versus* palladium

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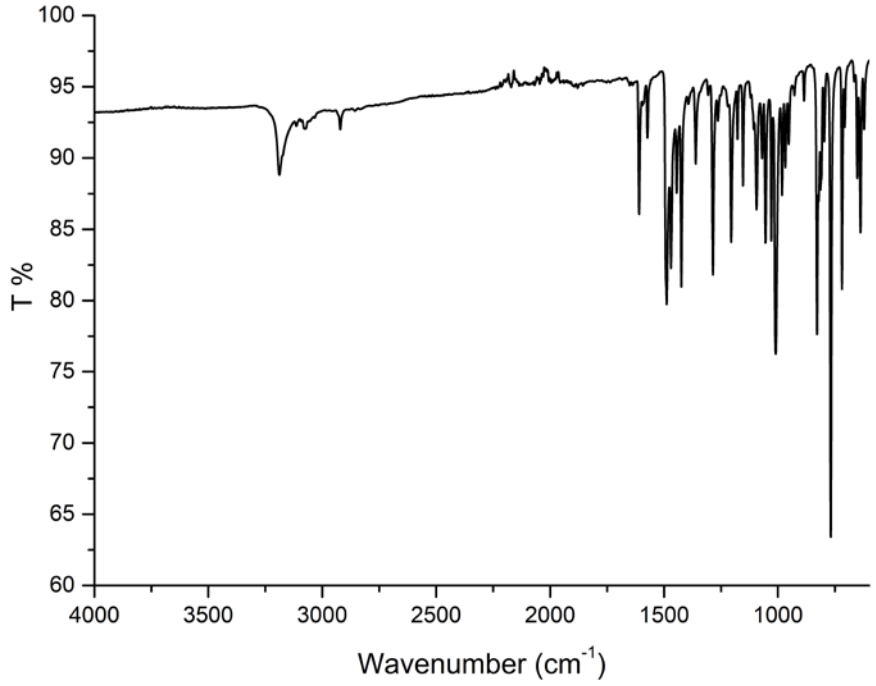

Fig. S1 Infrared spectrum (diamond/ZnSe ATR) of **1**.

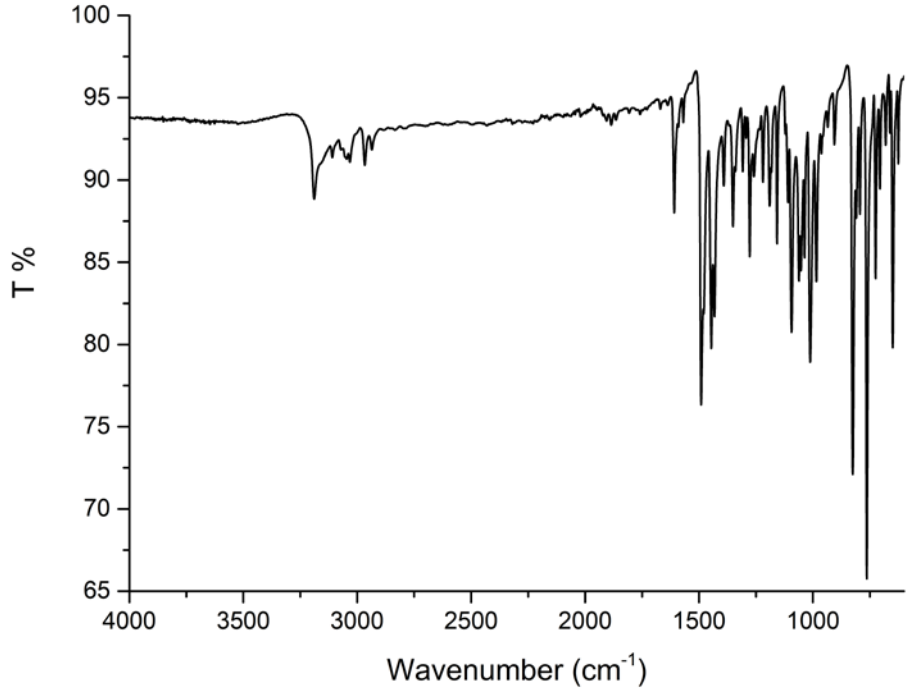

Fig. S2 Infrared spectrum (diamond/ZnSe ATR) of **2**.

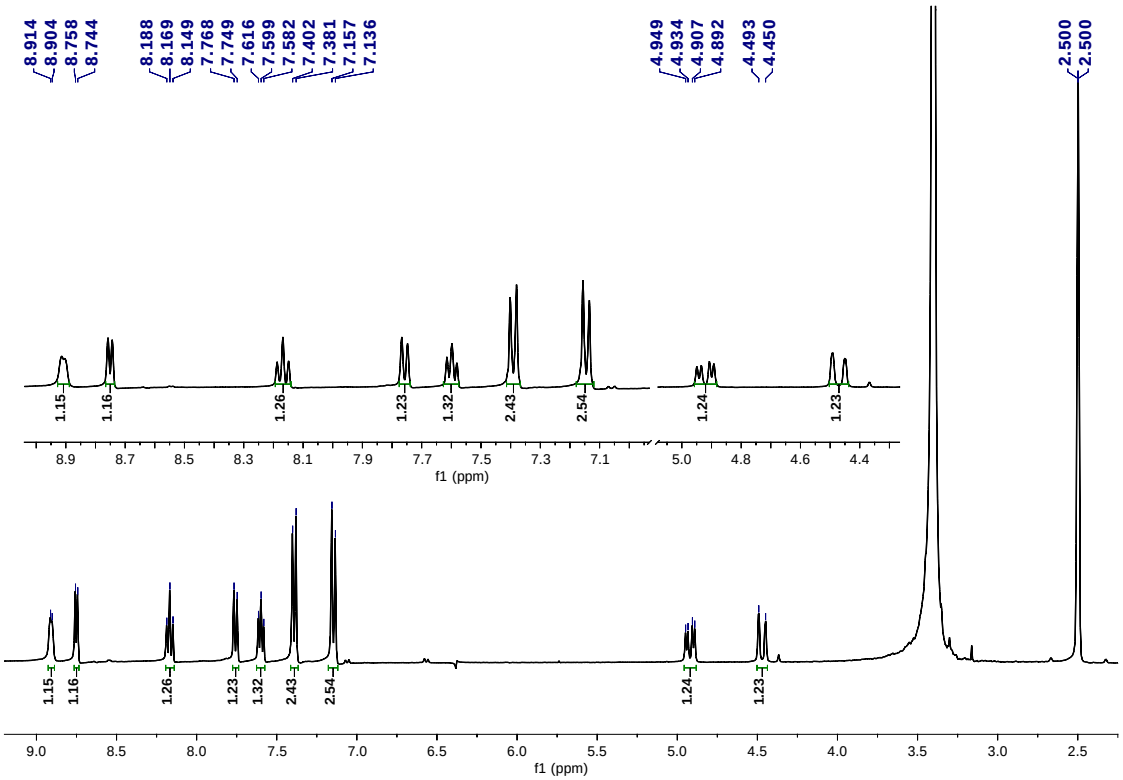

Fig. S3 ^{1}H NMR spectrum of **2** in DMSO-d_6 and zoom of the region 9.0–4.4 ppm (inset).

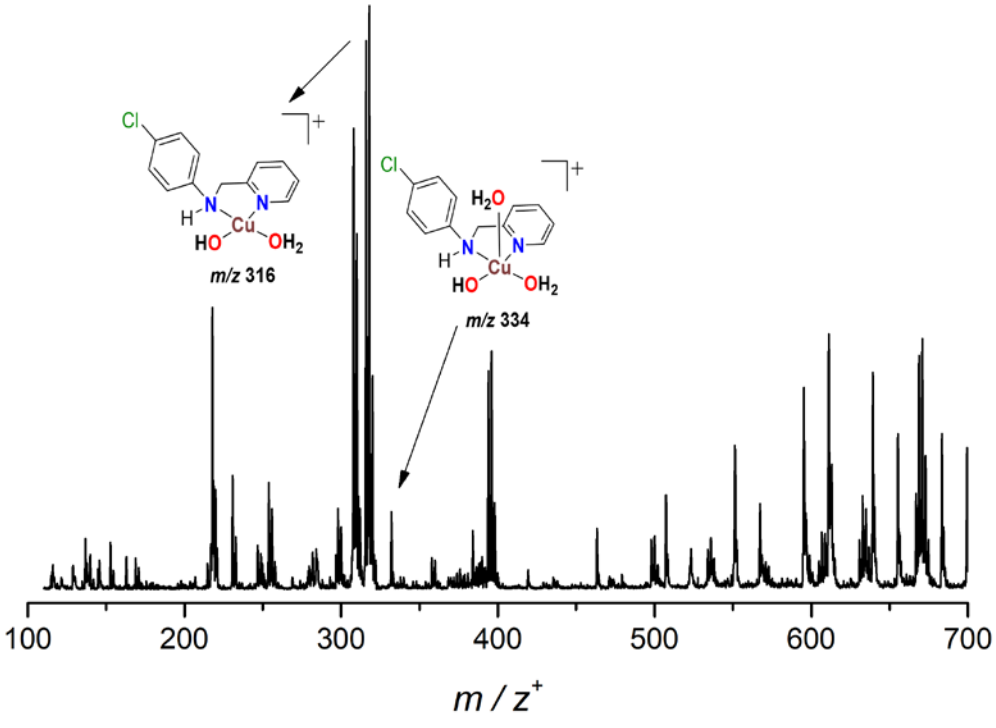

Fig. S4 ESI-MS spectrum of **1**.

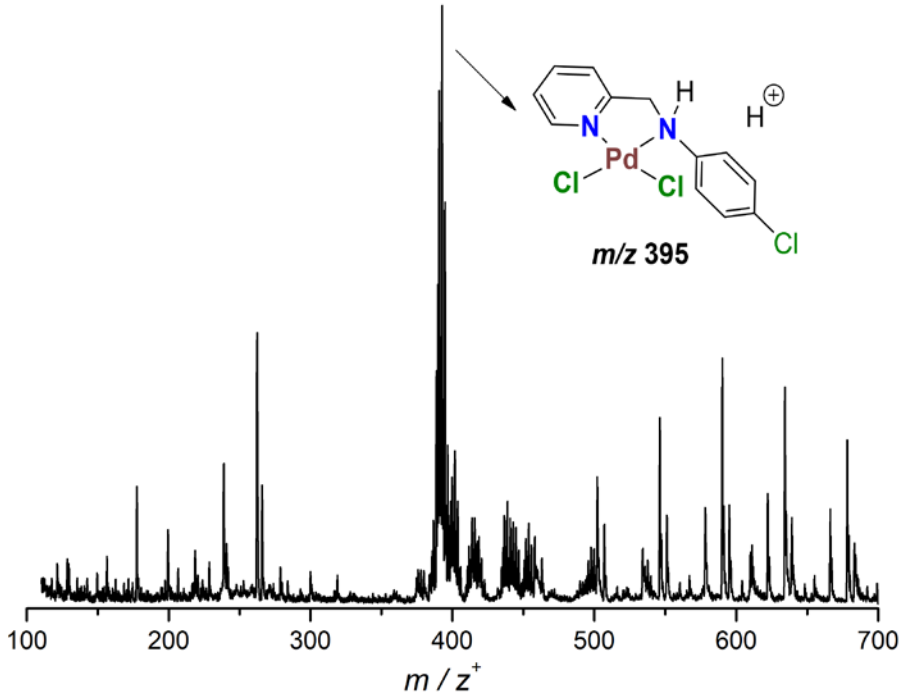

Fig. S5 ESI-MS spectrogram of **2**.

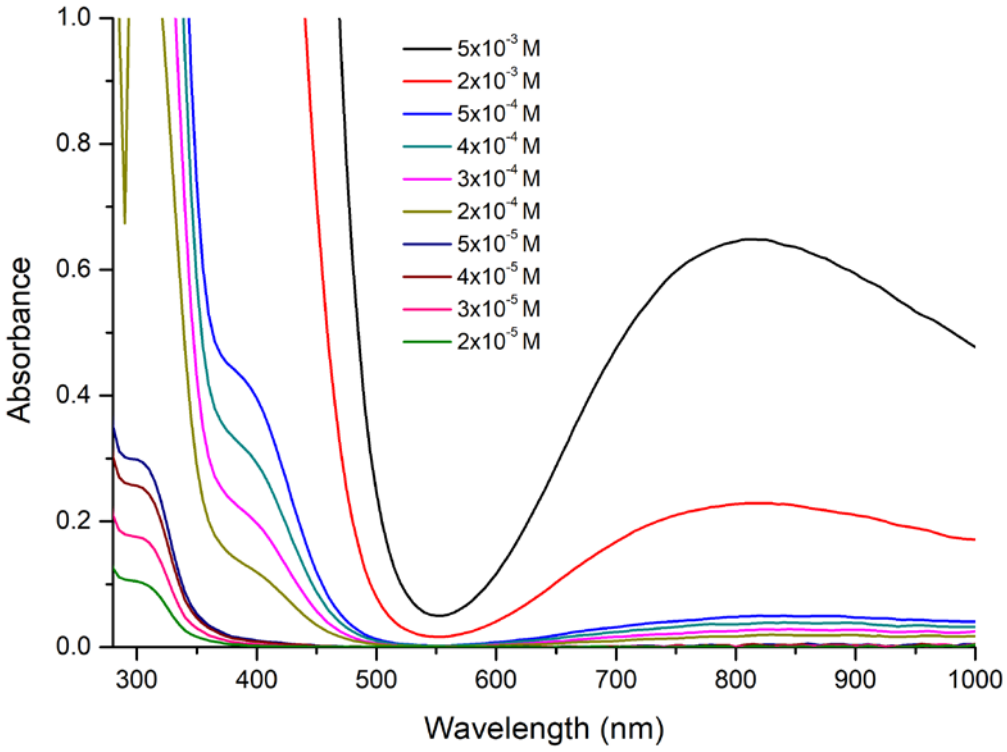

Fig. S6 UV-Visible spectra of **1** in DMSO at different concentrations.

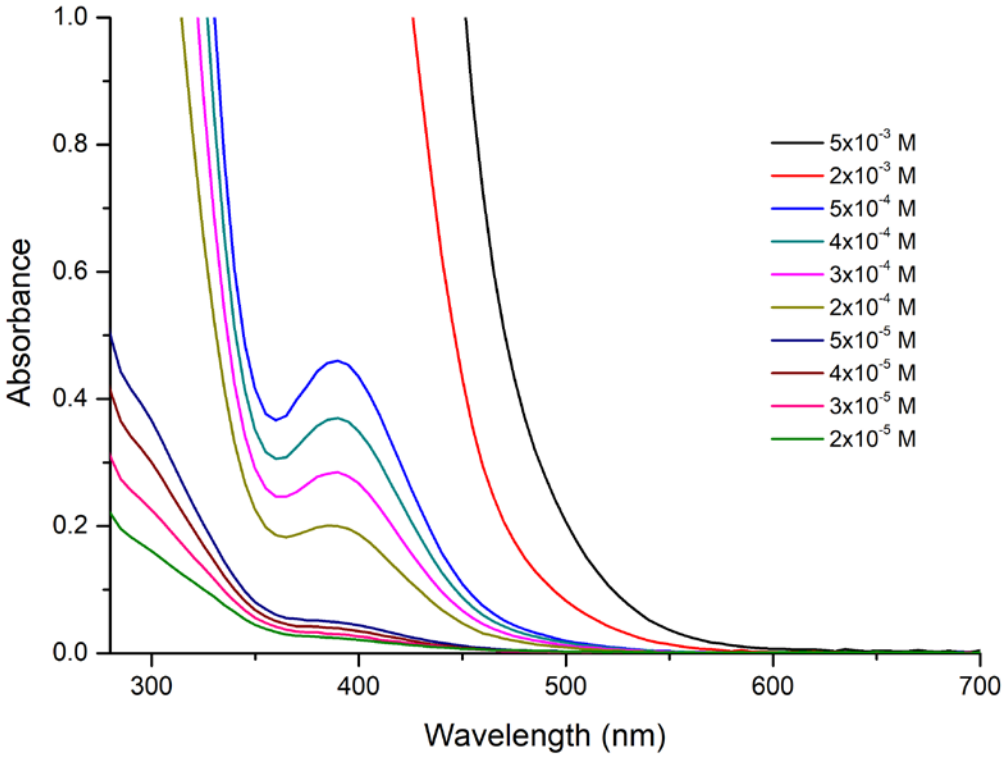

Fig. S7 UV-Visible spectra of **2** in DMSO at different concentrations.

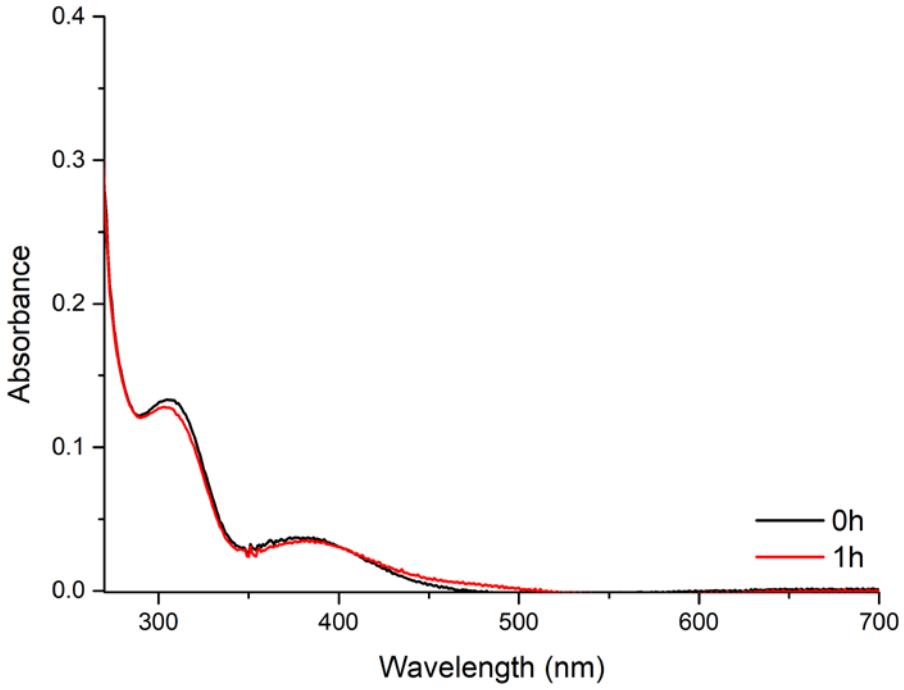

Fig. S8 UV-Visible monitoring of **1** (50 µM) in cacodylate–NaCl buffer containing 1% DMSO during 1 h at room temperature.

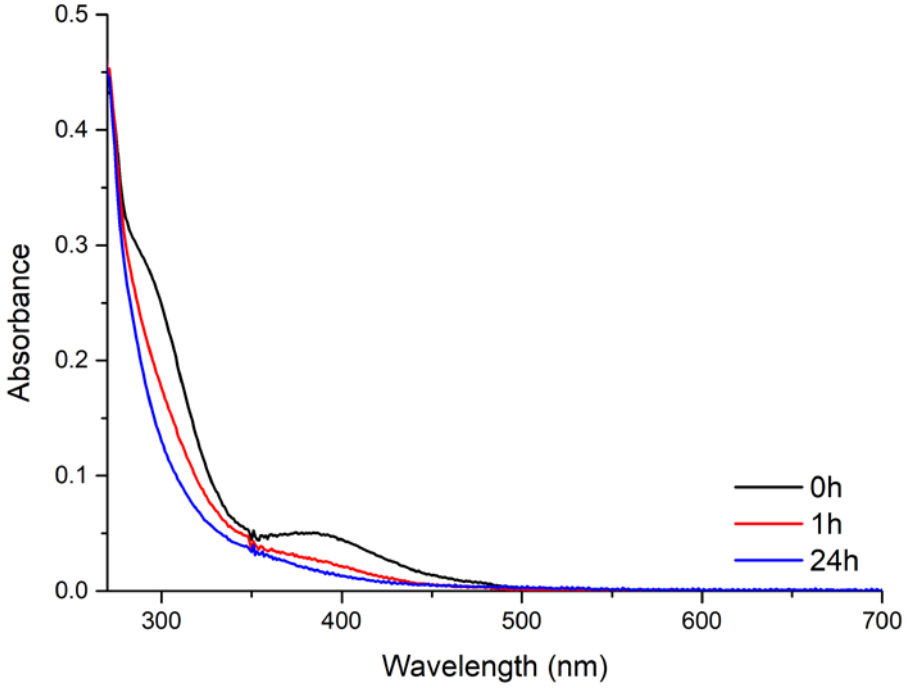

Fig. S9 UV-Visible monitoring of **2** (50 μM) in cacodylate–NaCl buffer containing 1% DMSO during 24 h at room temperature.

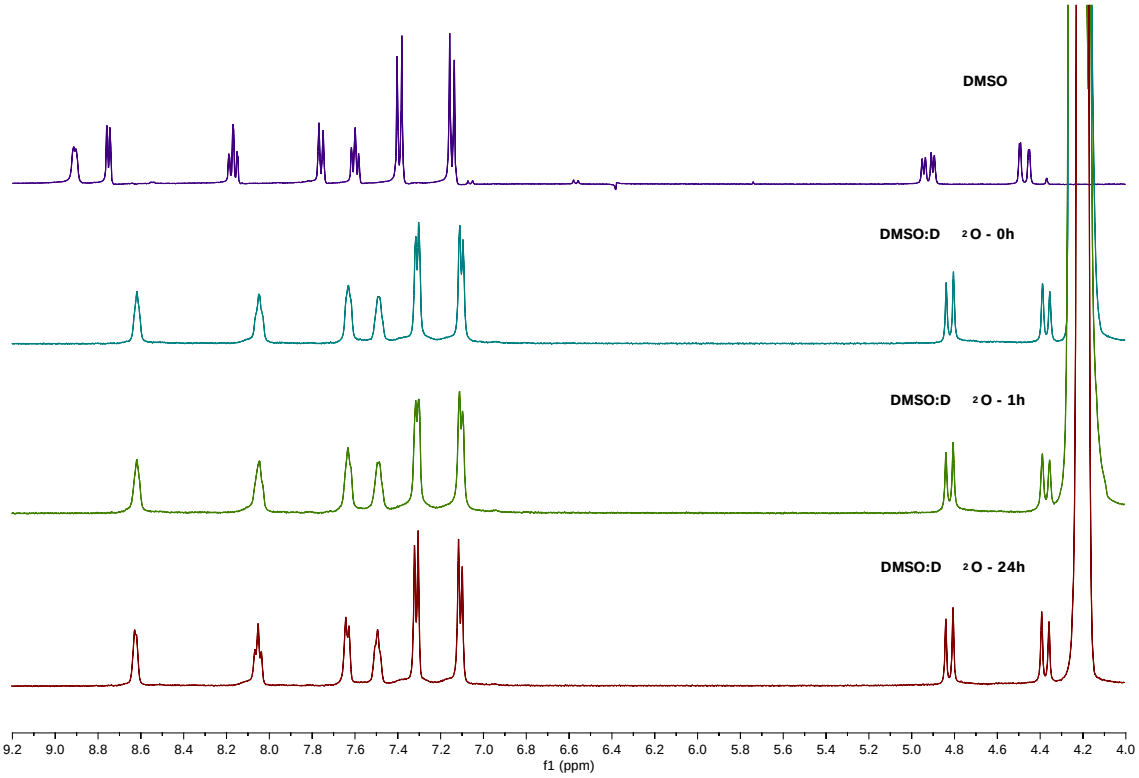

Fig. S10 ^{1}H NMR spectra of **2** in DMSO and DMSO/D_2O after 0, 1 and 24 h at 37 ºC.

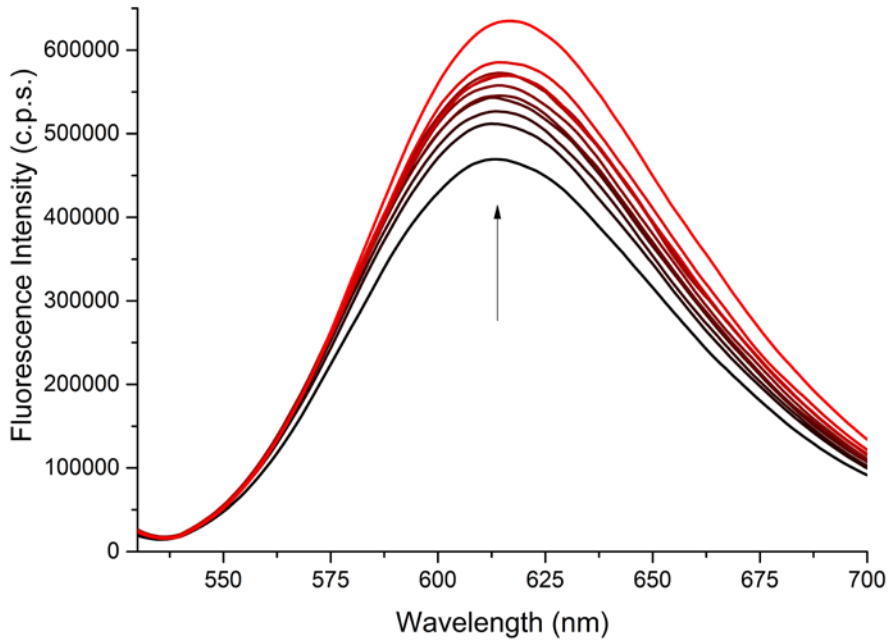

Fig. S11 Fluorescence emission spectra of the DNA–EB complex in the absence and presence of increasing amounts of complex **1**, [EB] = 75 μM, [DNA] =15 μM, [Complex] = 0–50 μM, λ_{ex} = 514 nm.

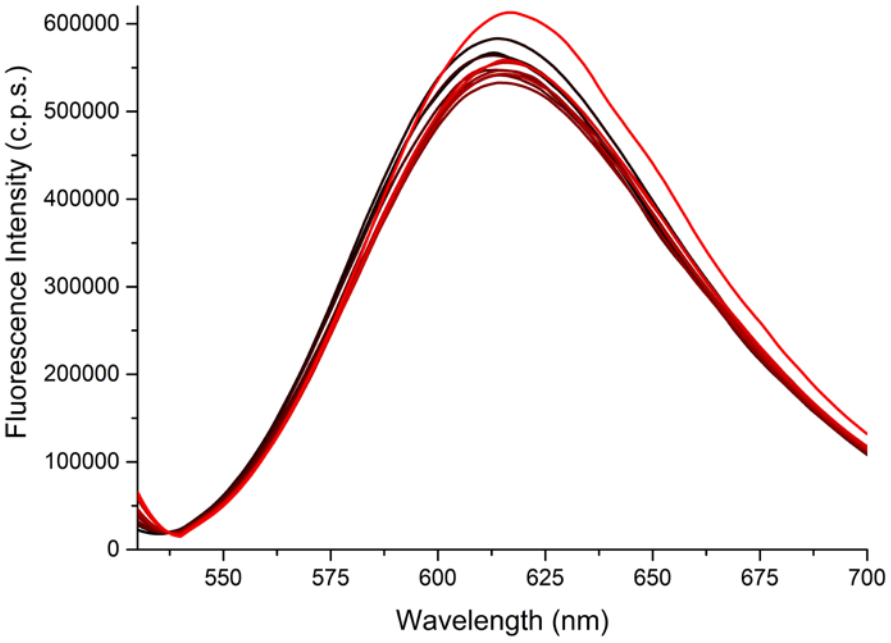

Fig. S12 Fluorescence emission spectra of the DNA–EB complex in the absence and presence of increasing amounts of complex **2**, [EB] = 75 μM, [DNA] =15 μM, [Complex] = 0–50 μM, λ_{ex} = 514 nm.

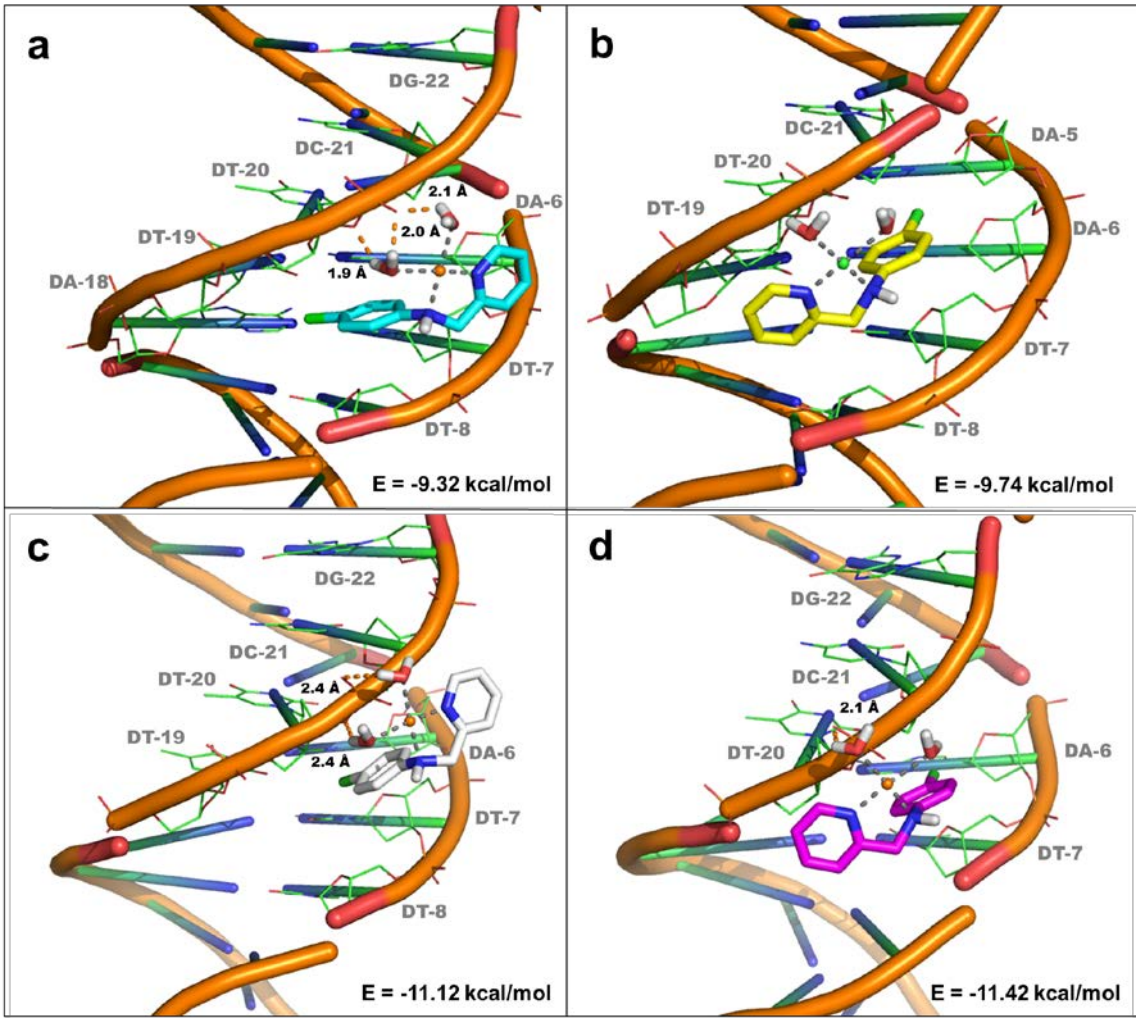

Fig. S13 Binding-mode analysis of the two enantiomers of $[Cu(CPYA)(H_2O)_2]^{2+}$ (**1a**) (top) and $[Pd(CPYA)(H_2O)_2]^{2+}$ (**2a**) (bottom) with the DNA (PDB: 1BNA). The enantiomers **1a*R***, **1a*S***, **2a*R*** and **2a*S*** are shown in cyan, yellow, white and pink, respectively. Hydrogen bonds are colored in orange. Metal-ligand bonds are colored in gray.

Table S1 Summary of crystal data, collection and refinement of complexes [Cu(CPYA)Cl_2] (**1**) and [Pd(CPYA)Cl_2] (**2**)**.**

	*Complex **1***	*Complex **2***
Empirical formula	$C_{12}H_{11}Cl_3CuN_2$	$C_{12}H_{11}Cl_3N_2Pd\cdot CH_3CN$
Formula weight ($g.mol^{-1}$)	353.12	437.03
Crystal system	Monoclinic	Monoclinic
Space group	$P2_1/c$	$P2_1/c$
Temperature (K)	298	298
Wavelength	Mo Kα	Mo Kα
Unit cell dimensions (Å,º)	a = 12.2234 (13) b = 14.8800 (14) c = 7.7366 (6) α = 90° β = 105.775 (4)° γ = 90°	a = 10.744 (4) b = 9.369 (3) c = 16.417 (6) α = 90° β = 92.169 (13)° γ = 90°
Volume ($Å^3$)	1354.2 (2)	1651.4 (10)
Z	4	4
D_x (Mg/m^3)	1.732	1.758
Absorption coefficient (mm^{-1})	2.19	1.60
F(000)	708	864
Index ranges	h = −14 → 14 k = −17 → 17 l = −9 → 9	h = −12 → 12 k = −11 → 11 l = −19 → 19
R_{int}	0.036	0.073
Reflections collected	38635	26680
Independent reflections	2380	2887
Reflections observed [I>2σ(I)]	2102	2525
Θ range for data collection	3.1 to 25.0º	2.5 to 25.0º
R [$F^2>2\sigma F^2$]	0.025	0.054
wR (F^2)	0.059	0.146
S	1.14	1.15
Parameters	168	191
Δρ min ($e\ Å^{-3}$)	−0.30	−1.37
Δρ max ($e\ Å^{-3}$)	0.44	1.92

Table S2 Selected bond lengths (Å) and angles (°) for complexes [Cu(CPYA)Cl_2] (**1**) and [Pd(CPYA)Cl_2] (**2**).

Atom labels	**1** (M = Cu)	**2** (M = Pd)
M—N1	2.087(2)	2.081(5)
M—N2	1.999(2)	2.040(5)
M—Cl1	2.2524(7)	2.2979(18)
M—Cl2	2.2645(7)	2.3142(17)
N1—M—N2	82.40(8)	82.64(19)
N1—M—Cl1	90.19(6)	90.43(14)
N1—M—Cl2	177.28(6)	175.73(14)
N2—M—Cl1	168.95(6)	172.64(14)
N2—M—Cl2	95.03(6)	93.99(14)
Cl1—M—Cl2	92.23(3)	93.04(6)