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A water-soluble Pd(II) complex with a terpyridine ligand: Experimental and molecular modeling studies of the interaction with DNA and BSA; and *in vitro* cytotoxicity investigations against five human cancer cell lines

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Table S1

Selected bond lengths and bond angles for 4'-(4-hydroxyphenyl)-2,2',6',2''-terpyridine (4-OHPh-tpy).

Bond lengths (Å)			
O1—C19	1.409 (6)	N1—C10	1.351 (6)
O1—H1	0.8200	C1—N2	1.334 (6)
N1—C6	1.334 (7)	N2—C5	1.343 (7)
Bond angles (°)			
C19—O1—H1	109.5	C5—N2—C1	118.0 (6)
C6—N1—C10	117.8 (5)	N1—C10—C9	122.8 (6)
N3—C11—C12	121.8 (7)	N1—C10—C11	116.0 (6)
N2—C1—C2	122.5 (6)	N1—C6—C7	122.2 (6)
N2—C1—C6	118.6 (6)	N1—C6—C1	116.8 (6)
C2—C1—C6	118.8 (6)	C15—N3—C11	116.3 (6)

Table S2

Selected bond lengths and bond angles for the Pd(II) complex.

Bond lengths (Å)			
Pd1-Cl1	2.290(3)	Pd1-N2	1.946(9)
Pd1-N1	2.020(9)	Pd1-N3	2.032(9)
Bond angles (°)			
N2—Pd1—N1	81.1(4)	N2—Pd1—Cl1	179.1(3)
N2—Pd1—N3	80.4(4)	N1—Pd1—Cl1	99.3(3)
N1—Pd1—N3	161.5(4)	N3—Pd1—Cl1	99.2(3)

Table S3

Hydrogen bond geometry (Å and °) for the Pd(II) complex.

D-H...A	d(D-H)	d(H...A)	d(D...A)	Angle DHA
O20-H20...Cl2	0.83(17)	2.14(17)	2.942(10)	160(17)
O1W-H11W...Cl2^{i}	0.82(16)	2.4(2)	2.950(11)	126(17)
O1W-H12W...O1W^{ii}	0.80(2)	2.04(10)	2.769(15)	151(20)
C2-H2...Cl1^{iii}	0.95	2.79	3.452(11)	128
C3-H3...Cl1^{iii}	0.95	2.84	3.468(11)	125
C4-H4...O20^{iv}	0.95	2.55	3.177(13)	123
C5-H5...Cl2^{v}	0.95	2.53	3.474(12)	171
C10-H10...Cl3^{i}	0.95	2.75	3.694(12)	174
C13-H13...Cl3^{i}	0.95	2.66	3.599(13)	171
C14-H14...Cl3^{vi}	0.95	2.82	3.769(14)	171
C22-H22...Cl3^{i}	0.95	2.68	3.611(12)	165

Symmetry operations: i x,y,z−1 ii −y+3/2,x,z iii −x+1,−y+1,−z+4 iv y,−x+3/2,z+2 v y,−x+3/2,z+1 vi −y+1,x−1/2,−z+2

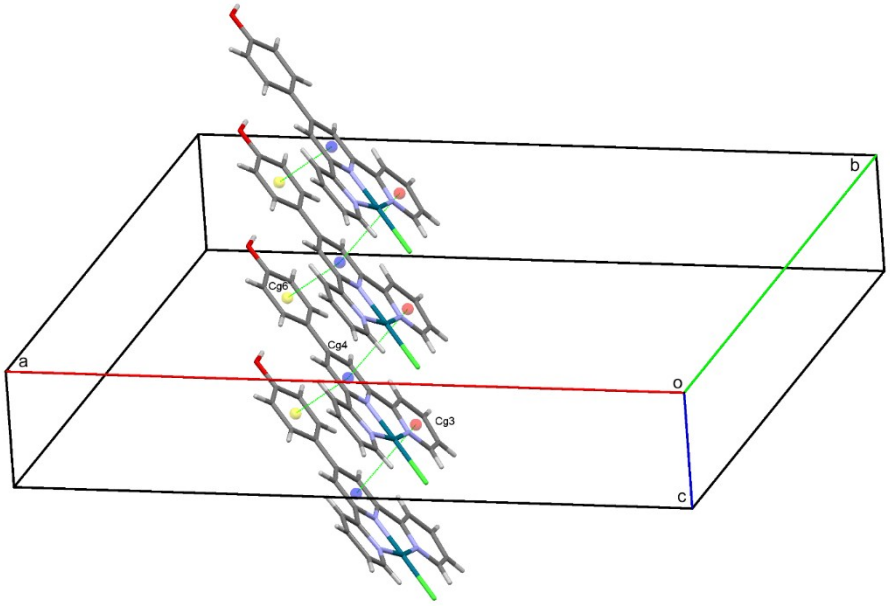

Fig. S1. Offset $\pi\cdots\pi$ stacking contacts, drawn as dotted green lines, for the Pd(II) complex. The ring centroids are shown as colored spheres: Cg3 N1, C2 , C3, C4, C 5, C6, red, Cg4 N2, C7, C68, C9, C10, C11, blue; and Cg6 C17, C18 C19, C20, C21, C22, yellow.

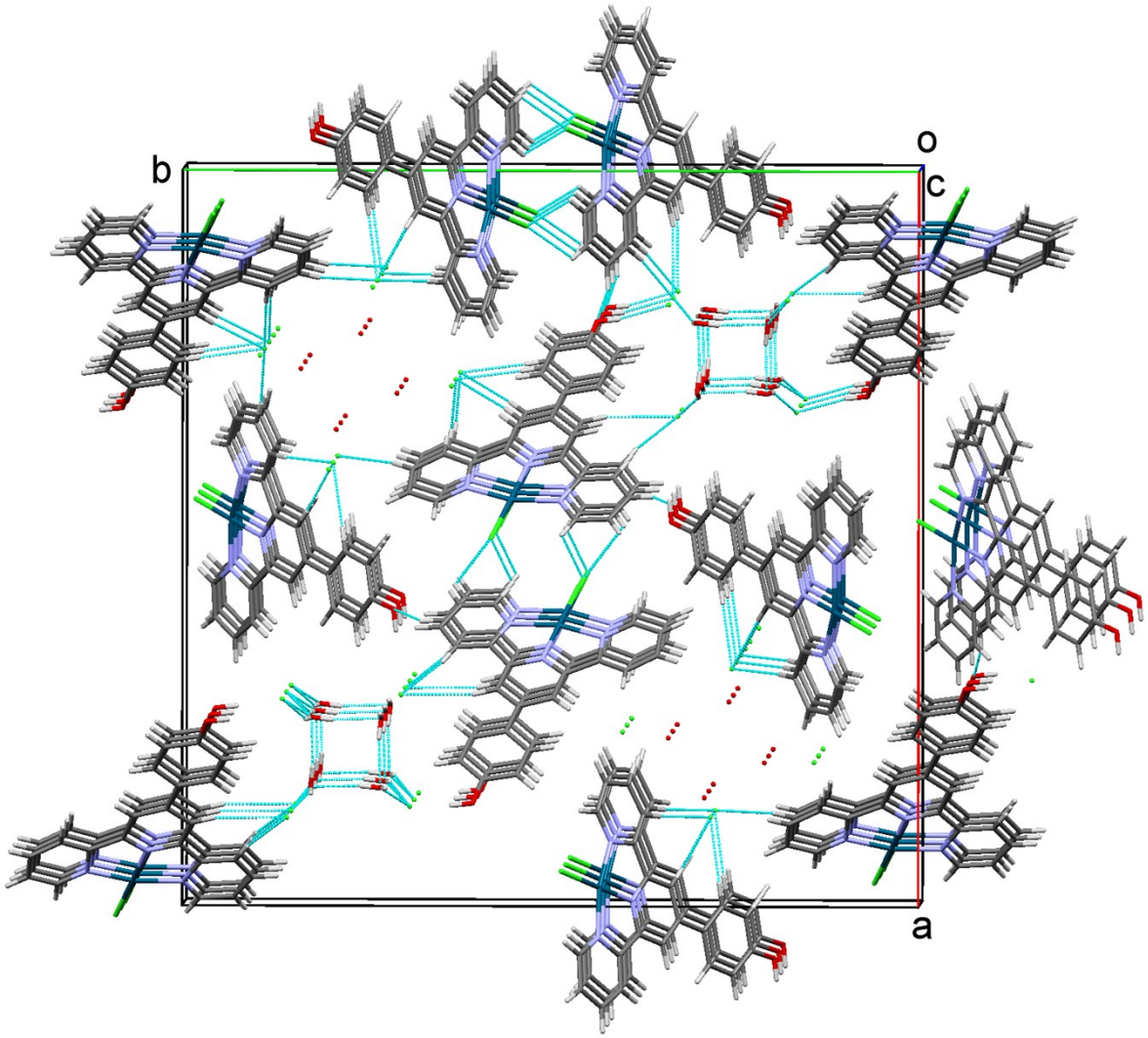

Fig. S2. Overall packing for the Pd(II) complex with hydrogen bonds drawn as dashed lines.

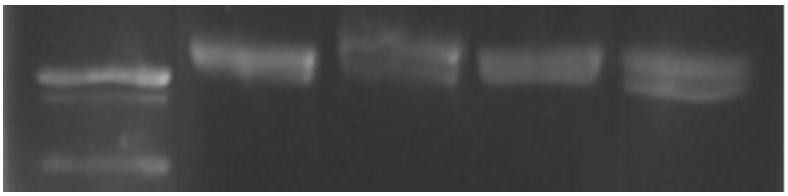

Fig. S3. Gel electrophoresis diagrams showing the cleavage of pUC57 DNA (0.01 M) by the Pd(II) complex in Tris-HCl buffer (pH = 7.2) at 37ºC for 3 h in the presence of NaN_3, DMSO and H_2O_2. Lane 1: DNA control; Lane 2: DNA + the complex (500 μM); Lane 3: DNA + the complex (500 μM) + NaN_3 (500 μM); Lane 4: DNA + the complex (500 μM) + DMSO (500 μM); and Lane 5: DNA + the complex (500 μM) + H_2O_2 (500 μM).

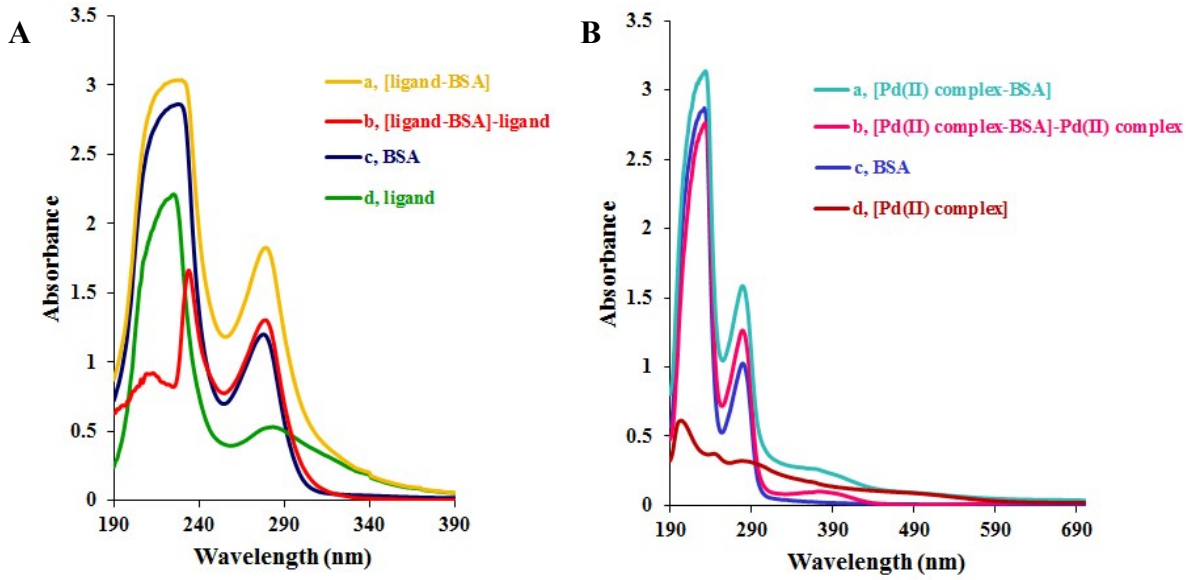

Fig. S4. (A) Electronic absorption spectra of BSA in the presence of the ligand (4-OHPh-tpy). (a) (yellow) The absorption spectra of the ligand-BSA system when the mole ratio is 1:1; (b) (red) the difference absorption spectra between the ligand-BSA system and the free ligand at the same concentration (c); (navy blue) the absorption spectra of BSA only; (d) (green) the absorption spectra of the free ligand only. **(B)** Electronic absorption spectra of BSA in the presence of the Pd(II) complex. (a) (blue-green) The absorption spectra of the BSA-complex system when the mole ratio is 1:1; (b) (pink) the difference absorption spectra between the BSA-complex system and the complex at the same concentration (c); (blue) the absorption spectra of BSA only; (d) (red) the absorption spectra of the complex only.

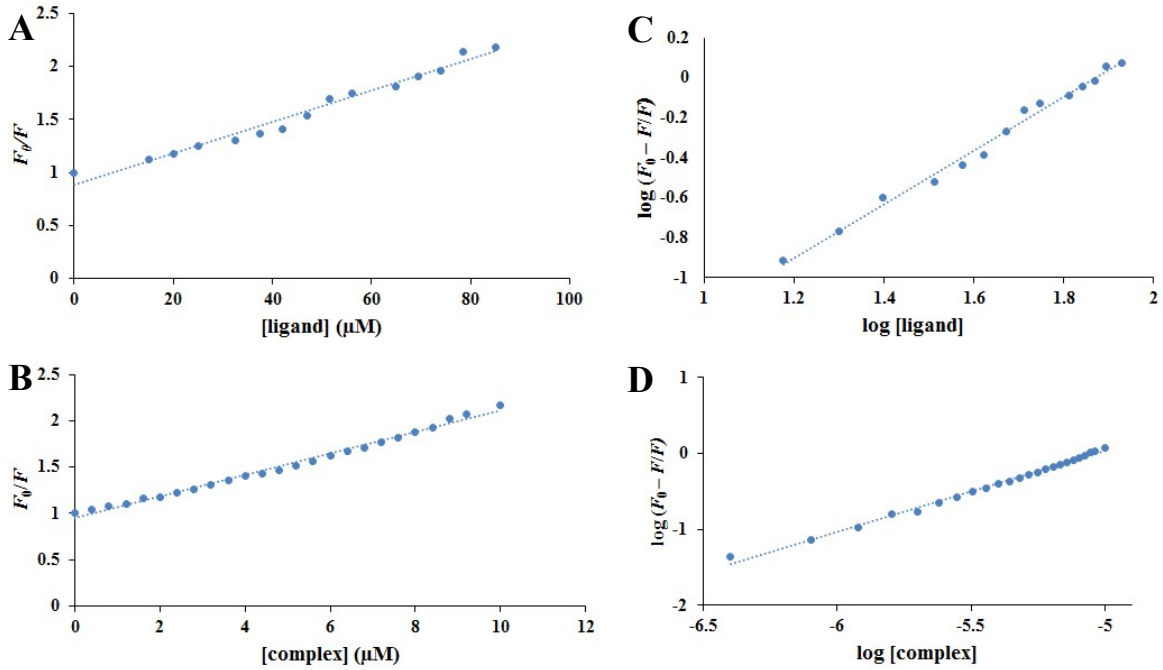

Fig. S5. Stern–Volmer plots for fluorescence quenching of BSA by the ligand (**A**) and the Pd(II) complex (**B**); Plot of log ($F_0 - F$)/F) *versus* log [ligand or complex] (**C** and **D**).

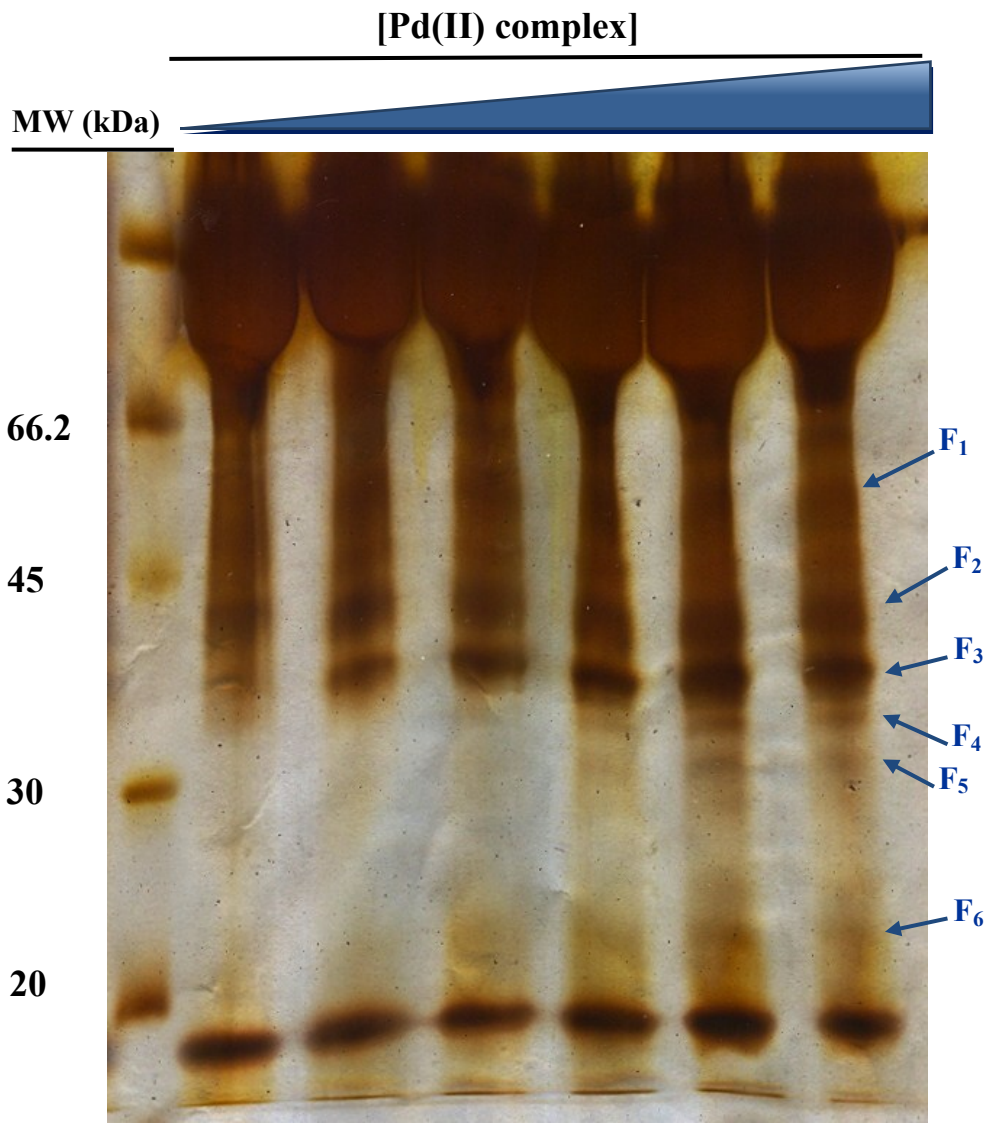

Fig. S6. BSA fragmentation by the Pd(II) complex in phosphate buffer (pH = 7.4) at 37 ºC for 1 h: Lane 1: control BSA (10 μM); Lane 2: BSA control + the complex (50 μM), Lane 3: BSA control + the complex (100 μM), Lane 4: BSA + the complex (200 μM), Lane 5: BSA + the complex (300 μM), and Lane 5: BSA + the complex (400 μM). The main cleavage products are indicated by the arrows F_1-F_6.

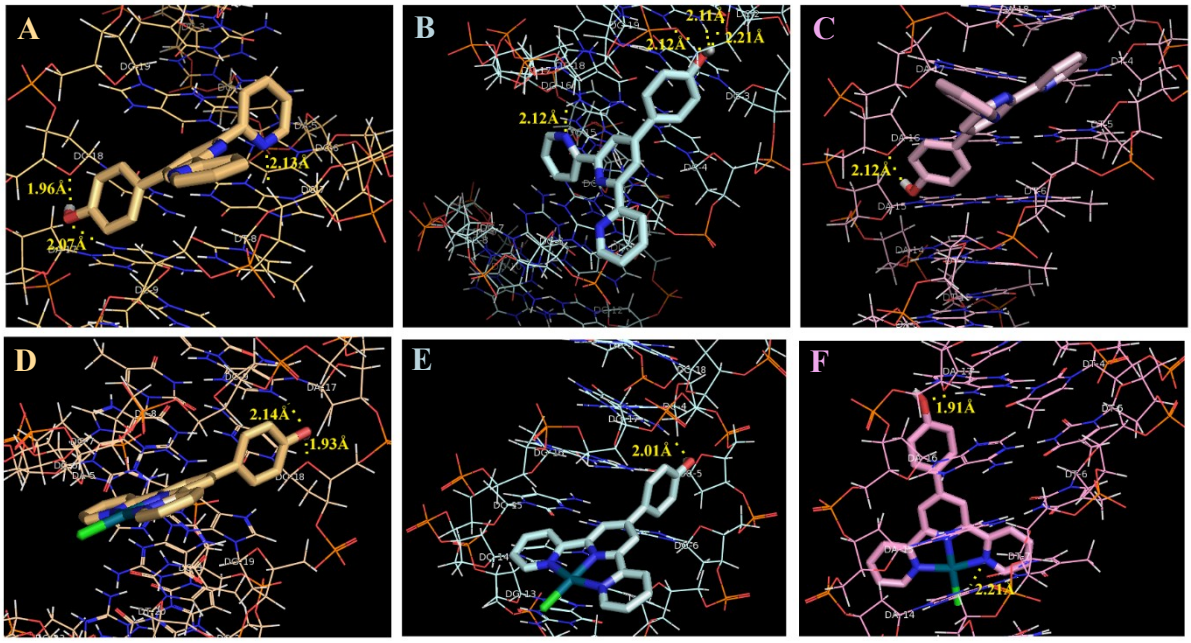

Fig. S7. The hydrogen bonding interaction between DNA and 4-OHPh-tpy (**A**, **B**, and **C**) or the Pd(II) complex (**D**, **E**, and **F**); a mixed sequence (**A** and **D**), GC-rich (**B** and **E**), and AT-rich (**C** and **F**).