Electronic Supplementary Information for

Synthesis, characterization, interaction with DNA and cytotoxicity of Pd(II) and Pt(II) complexes containing pyridine carboxylic acid ligands

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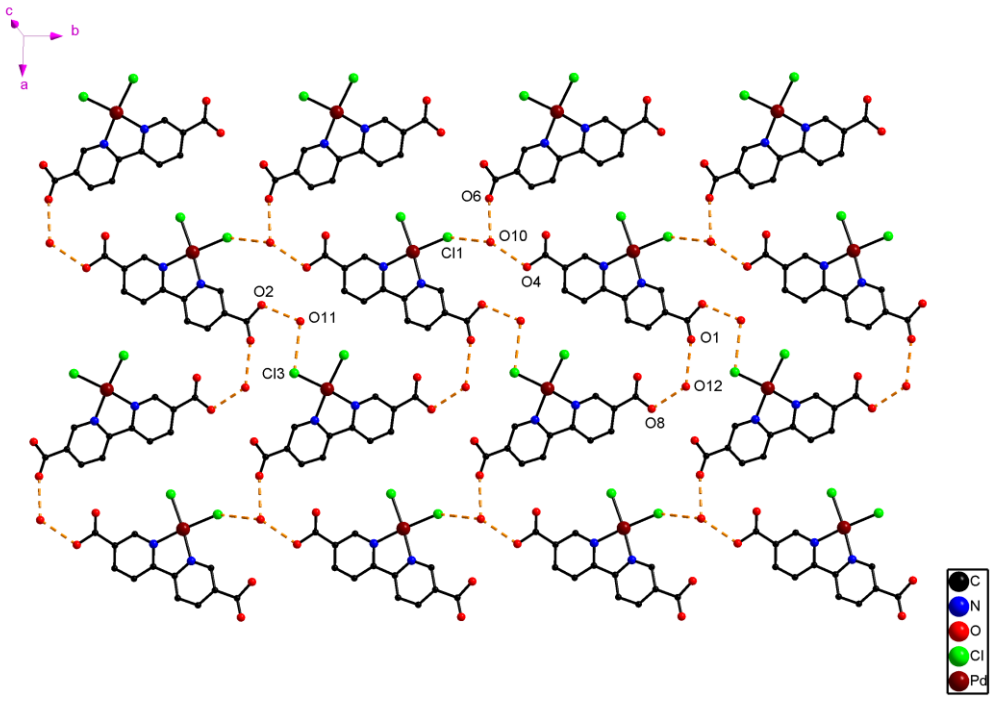

Fig. S1 Two-dimensional structure of complex **1** connected via hydrogen bond.

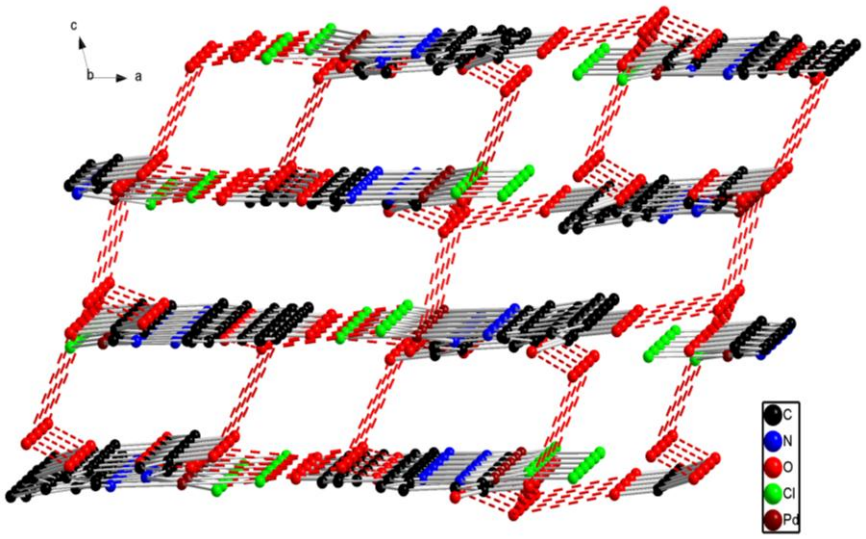

Fig. S2 Three-dimensional structure of complex **1** connected via hydrogen bond.

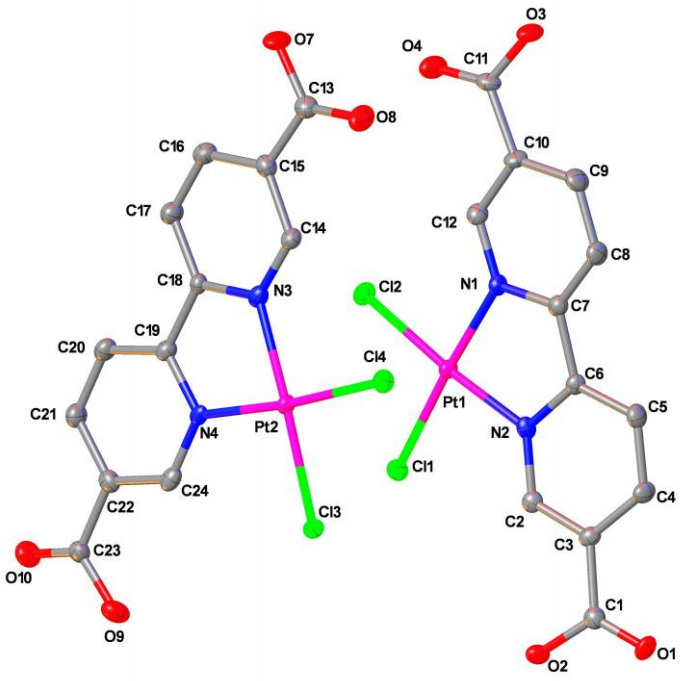

Fig. S3 Molecular structure of the complex **2**.

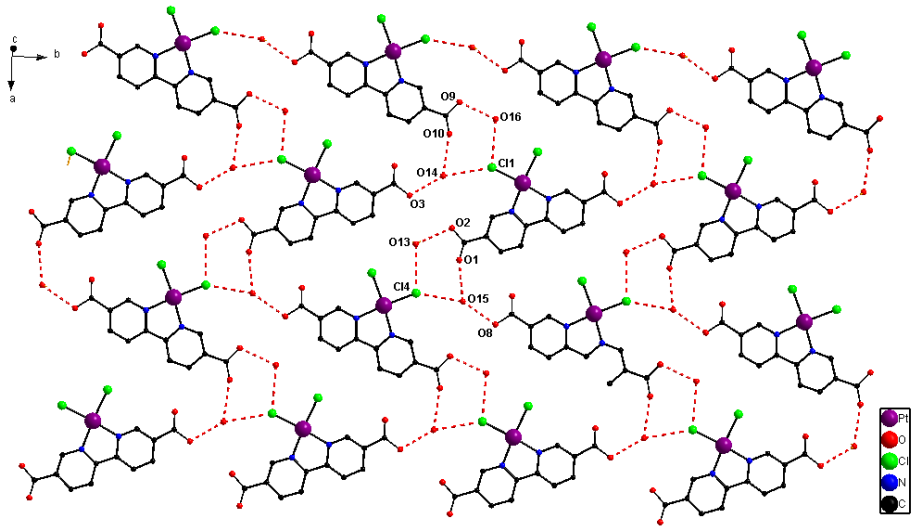

Fig. S4 Two-dimensional structure of complex **2** connected via hydrogen bond.

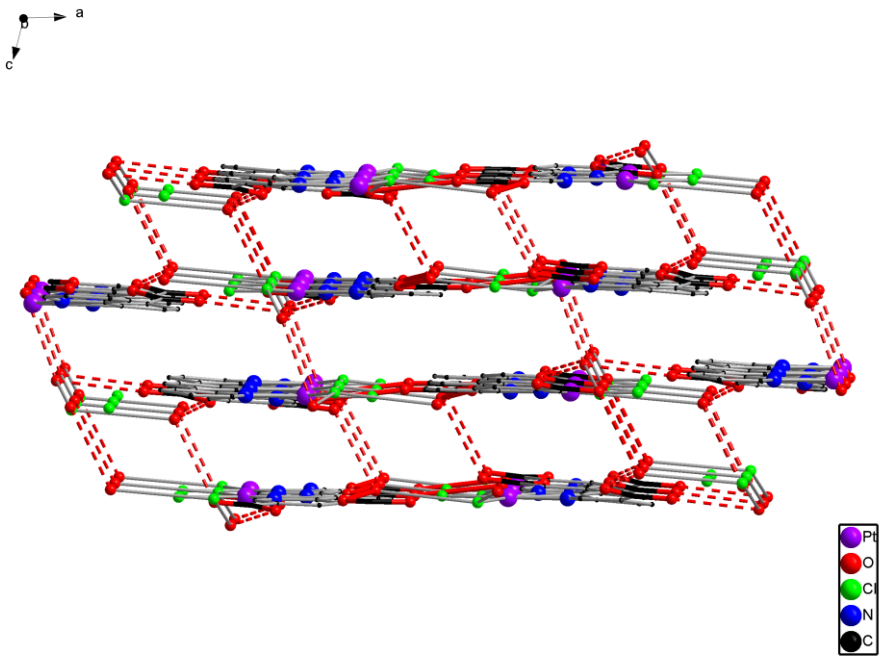

Fig. S5 Three-dimensional structure of complex **2** connected via hydrogen bond.

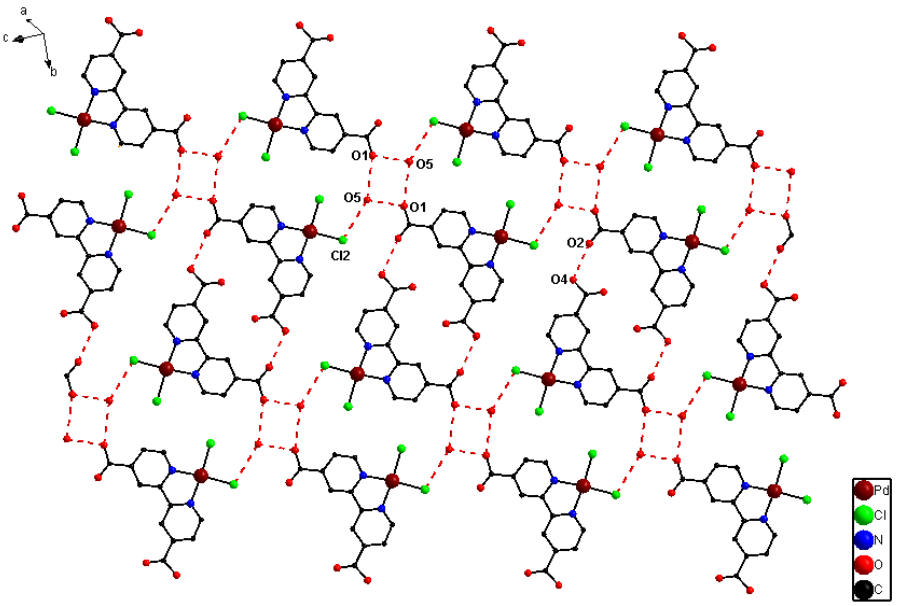

Fig. S6 Two-dimensional structure of complex **3** connected via hydrogen bond.

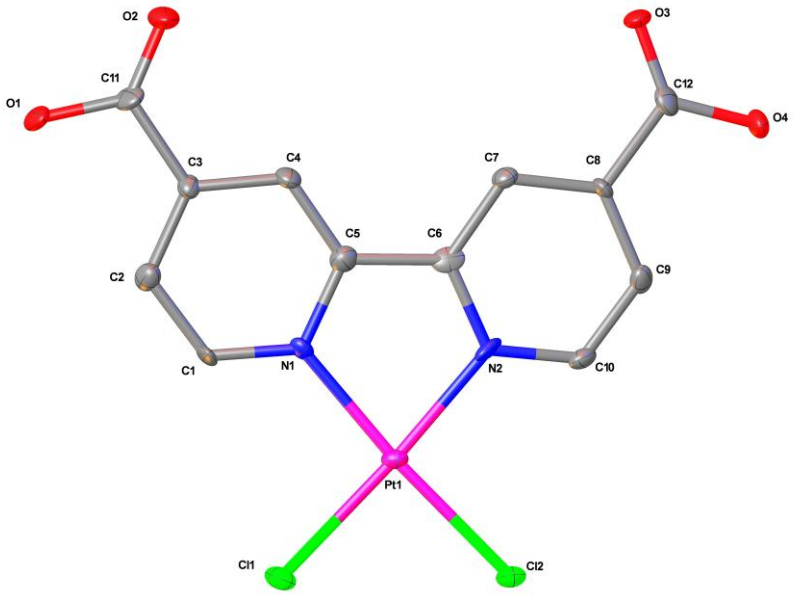

Fig. S7 Molecular structure of the complex **4**.

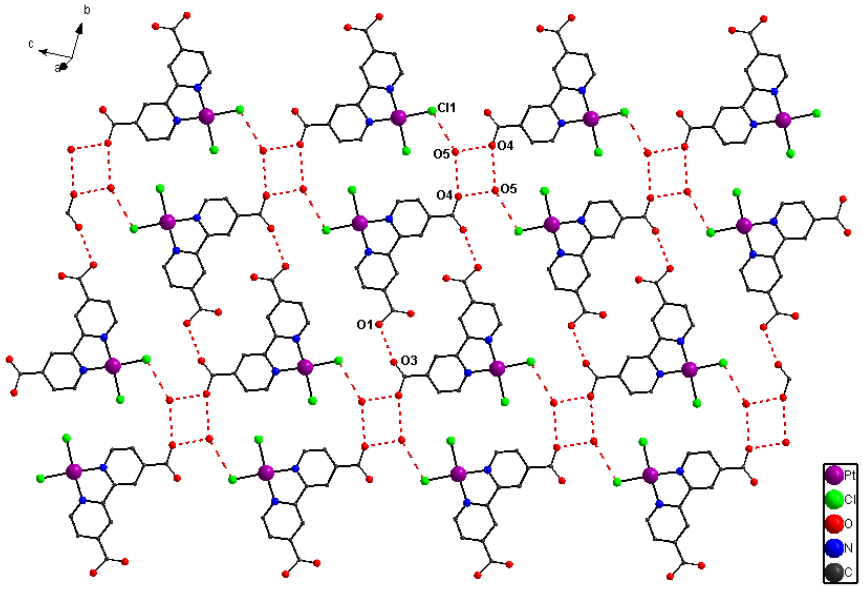

Fig. S8 Two-dimensional structure of complex **4** connected via hydrogen bond.

Table S1 Crystal data and refinement for complexes **1-4**.

	1	**2**	**3**	**4**
Empirical formula	$C_{12}H_{12}Cl_2N_2O_6Pd$	$C_{12}H_{12}Cl_2N_2O_6Pt$	$C_{12}H_{10}Cl_2N_2O_5Pd$	$C_{12}H_{10}Cl_2N_2O_5Pt$
Formula weight	457.54	546.23	439.52	528.21
Temperature (K)	293(2) K	293(2) K	293(2) K	293(2) K
Wavelength	0.71073 Å	0.71075 Å	0.71073 Å	0.71073 Å
Crystal system	Monoclinic,	Monoclinic,	Triclinic	Triclinic
Space group	P2(1)/c	P2(1)/c	P-1	P-1
a (Å)	16.780(3)	16.640(2)	7.2791(15)	7.3879(15)
b(Å)	13.895(3)	13.7906(18)	8.0941(16)	7.9746(16)
c(Å)	13.596(3)	13.6697(19)	12.513(3)	12.542(3)
Volume ($Å^3$)	3022.0(11)	3014.6(7)	698.8(2)	697.1(3)
Z	8	8	2	2
Density(calculated) (Mg/m^3)	2.011	2.407	2.089	2.517
Absorption coefficient (mm^{-1})	1.614	9.696	1.735	10.473
F(000)	1808	2064	432	496
θ Range for data collection (°)	1.94 to 27.53	3.10 to 25.02	2.88 to 25.01	2.63 to 25.01
Reflections collected/unique	24305/6938[R(int) = 0.0581]	18633/5314[R(int) = 0.0686]	5067/2443[R(int) = 0.0199]	4748/2452[R(int) = 0.0423]
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalent	Semi-empirical from equivalents	Semi-empirical from equivalent
Refinement method	Full-matrixleast-squares on F^2	Full-matrixleast-squares on F^2	Full-matrixleast-squares on F^2	Full-matrixleast-squares on F^2
Data/restraints/parameters	6938 / 14 / 447	5314 / 9 / 421	2443 / 3 / 201	2452 / 3 / 201
Goodness-of-fit on F^2	1.051	1.109	1.136	1.021
Final R indices [$I > 2\sigma(I)$]	R1 = 0.0406, wR2 = 0.0817	R1 = 0.0521, wR2 = 0.0863	R1= 0.0224, wR2 = 0.0625	R1 = 0.0355, wR2 = 0.0771
R indices (all data)	R1 = 0.0581, wR2 = 0.0893	R1 = 0.0765, wR2 = 0.0925	R1 = 0.0255, wR2 = 0.0637	R1 = 0.0394, wR2 = 0.0788
Largest diff. peak and hole (e $Å^{-3}$)	0.858 and -1.353	1.779 and -0.903	1.584 and -0.486	1.688 and -2.142
Crystallographic Data Center as supplementary publication number CCDC	733797	733798	729229	729232

Table S2 Selected bond lengths (Å) and angles (º) for complex **1** and **2** together with the calculated values by DFT.

complex **1**			complex **2**		
	Exp. value	6-311G(d, p)		Exp. value	6-311G(d, p)
Pd(1)-Cl(1)	2.2953(10)	2.3267	Pt(2)-Cl(3)	2.283(3)	2.3455
Pd(1)-Cl(2)	2.2910(9)	2.3235	Pt(2)-Cl(4)	2.274(3)	2.3455
Pd(1)-N(1)	2.025(3)	2.0962	Pt(2)-N(3)	1.998(8)	2.0560
Pd(1)-N(2)	2.022(3)	2.0969	Pt(2)-N(4)	1.999(8)	2.0560
O(1)-C(1)	1.202(4)	1.2056	O(7)-C(13)	1.199(15)	1.2020
O(2)-C(1)	1.336(4)	1.3433	O(8)-C(13)	1.292(15)	1.3524
O(3)-C(12)	1.221(4)	1.2020	O(9)-C(23)	1.249(15)	1.2020
O(4)-C(12)	1.319(5)	1.3524	O(10)-C(23)	1.227(15)	1.3524
Cl(2)-Pd(1)-Cl(1)	89.23(3)	91.58	Cl(3)-Pt(2)-Cl(4)	88.75(10)	90.32
N(1)-Pd(1)-Cl(1)	95.74(9)	94.79	N(3)-Pt(2)-Cl(4)	176.3(3)	174.63
N(1)-Pd(1)-Cl(2)	175.02(9)	173.64	N(3)-Pt(2)-Cl(3)	94.9(3)	95.05
N(2)-Pd(1)-Cl(1)	176.17(8)	173.55	N(4)-Pt(2)-Cl(4)	96.1(2)	95.05
N(2)-Pd(1)-Cl(2)	94.36(8)	94.87	N(4)-Pt(2)-Cl(3)	175.2(3)	174.63
N(2)-Pd(1)-N(1)	80.67(12)	78.76	N(3)-Pt(2)-N(4)	80.3(3)	79.58
O(2)-C(1)-O(1)	123.8(4)	124.06	O(7)-C(13)-O(8)	124.5(11)	123.57
O(3)-C(12)-O(4)	123.0(4)	123.57	O(9)-C(23)-O(10)	124.8(13)	123.57
Cl(2)-Pd(1)-Cl(1)	89.56(4)	91.40	Cl(2)-Pt(1)-Cl(1)	89.14(10)	90.06
N(1)-Pd(1)-Cl(1)	94.45(7)	94.81	N(1)-Pt(1)-Cl(2)	94.9(3)	95.09
N(1)-Pd(1)-Cl(2)	175.99(6)	173.78	N(1)-Pt(1)-Cl(1)	176.0(3)	174.85
N(2)-Pd(1)-Cl(2)	95.40(7)	94.82	N(2)-Pt(1)-Cl(2)	175.7(2)	174.85
N(2)-Pd(1)-Cl(1)	174.36(7)	173.78	N(2)-Pt(1)-Cl(1)	95.1(2)	95.09
N(2)-Pd(1)-N(1)	80.58(9)	78.97	N(2)-Pt(1)-N(1)	80.8(2)	79.75
O(2)-C(11)-O(1)	124.4(3)	123.80	O(2)-C(1)-O(1)	125.3(7)	123.74
O(3)-C(12)-O(4)	124.7(3)	123.80	O(3)-C(11)-O(4)	124.7(7)	123.74

Table S3 Selected bond lengths (Å) and angles (º) for complex **3** and **4** together with the calculated values by DFT.

complex **3**			complex **4**		
	Exp. value	6-311G(d, p)		Exp. value	6-311G(d, p)
Pd(1)-Cl(1)	2.2974(10)	2.3286	Pt(1)-Cl(1)	2.299(2)	2.3502
Pd(1)-Cl(2)	2.2957(10)	2.3286	Pt(1)-Cl(2)	2.2982(19)	2.3502
Pd(1)-N(1)	2.010(2)	2.0909	Pt(1)-N(1)	2.005(6)	2.0497
Pd(1)-N(2)	2.020(2)	2.0909	Pt(1)-N(2)	2.000(6)	2.0497
O(1)-C(11)	1.315(3)	1.3460	O(1)-C(11)	1.322(9)	1.3466
O(2)-C(11)	1.207(4)	1.2045	O(2)-C(11)	1.213(9)	1.2048
O(3)-C(12)	1.198(3)	1.2045	O(3)-C(12)	1.214(9)	1.3466
O(4)-C(12)	1.334(3)	1.3460	O(4)-C(12)	1.323(9)	1.2048

Table S4 HOMO and **LUMO** energies of complexes **1**-**4**.

	1	2	3	4
E_{HOMO}(a.u.)	-0.2627	-0.2471	-0.2634	-0.2487
E_{LUMO}(a.u.)	-0.1218	-0.1237	-0.1180	-0.1196
$\Delta E_{LUMO-HOMO}$(a.u.)	0.1409	0.1234	0.1454	0.1291