Supporting Information

Discovery of Pt (II) complexes based on terpyridine skeleton and study of their antiproliferative activity against pancreatic cancer cells

Ling Wang [a], Siying Chong [d], Shuangyan Wu[a], Yaguang Sun[a], Ying Zhang*[a], Chiyu Sun*[c] Mingchang Zhu*[a] [b]

[a] International Key Laboratory of Liaoning Inorganic Molecule-Based Chemical and Department of Coordination Chemistry, Shenyang University of Chemical Technology, Shenyang, 110142, P.R. China

[b] College of Environmental and Safety Engineering, Shenyang University of Chemical Technology, Shenyang, Liaoning, 110142, China

[c] Department of Pharmacology, Shenyang Medical College, Shenyang, 110034, PR China

[d] Liaoning Medical Device Test Institute, Liaoning Inspection, Examination and Certification Centre, Shenyang, Liaoning, China

**Corresponding author Email: zhangy621@syuct.edu.cn (Ying Zhang); mczhu@syuct.edu.cn (Mingchang Zhu); chiyusun@symc.edu.cn (Chiyu Sun)*

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Table S1 Crystallographic data and structure refinement parameters for CPT-Pt.

Identification code	CPT-Pt
Empirical formula	$C_{28}H_{27}Cl_4N_4O_3Pt_{1.5}$
Formula weight	242.29
Temperature/K	150(2)
Crystal system	triclinic
Space group	P-1
a/Å	8.0091(3)
b/Å	11.5449(4)
c/Å	16.7769(6)
α/°	93.224(2)
β/°	101.807(2)
γ/°	98.825(2)
Volume/Å^3	1494.30(9)
Z	17
ρ_{calc}g/cm^3	4.577
μ/mm^{-1}	39.754
F(000)	1734.0
Crystal size/mm^3	0.220 × 0.200 × 0.180
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	4.176 to 52.77
Index ranges	-10 ≤ h ≤ 10, -14 ≤ k ≤ 14, -20 ≤ l ≤ 20
Reflections collected	37057
Independent reflections	6097 [R_{int}= 0.0777, R_{sigma}= 0.0488]
Data/restraints/parameters	6097/64/387
Goodness-of-fit on F^2	0.975
Final R indexes [I>=2σ (I)]	R_1= 0.0339, wR_2= 0.0833
Final R indexes [all data]	R_1= 0.0525, wR_2= 0.0947
Largest diff. peak/hole / e Å^{-3}	1.20/-0.68

Table S2 Selected bond lengths(Å) for compound CPT-Pt.

Atom	Length/Å	Atom	Length/Å
C1-N1	1.342(9)	C19-N4	1.380(9)
C1-C2	1.372(11)	C19-C20	1.422(9)
C2-C3	1.381(10)	C20-C21	1.367(9)
C3-C4	1.377(10)	C22-N4	1.465(9)
C4-C5	1.371(10)	C22-C23	1.496(12)
C5-N1	1.374(9)	C23-C24	1.501(14)
C5-C6	1.490(9)	C24-C25	1.472(12)
C6-N2	1.345(8)	C24-C27	1.498(13)
C6-C7	1.380(9)	C25-C26	1.516(11)
C7-C8	1.398(9)	C26-N4	1.434(10)
C8-C9	1.408(9)	C27-O1A	1.199(13)
C8-C16	1.469(9)	C27-O2B	1.233(13)
C9-C10	1.383(9)	C27-O1B	1.283(14)
C10-N2	1.352(8)	C27-O2A	1.271(15)
C10-C11	1.489(9)	C28-O3	1.353(13)
C11-N3	1.362(9)	Cl1-Pt1	2.3022(18)
C11-C12	1.372(10)	Cl2-Pt2	2.3206(17)
C12-C13	1.408(10)	Cl3-Pt2	2.3105(16)
C13-C14	1.374(11)	Cl4-Pt2	2.3252(16)
C14-C15	1.369(11)	N1-Pt1	2.016(6)
C15-N3	1.349(9)	N2-Pt1	1.927(5)
C16-C17	1.404(9)	N3-Pt1	2.019(6)
C16-C21	1.405(9)	Pt2-Cl3^{1}	2.3105(16)
C17-C18	1.363(10)	Pt2-Cl2^{1}	2.3207(17)
C18-C19	1.410(10)	Pt2-Cl4^{1}	2.3252(16)

Table S3 Selected angles (°) for compound CPT-Pt.

Atom	Angle/°	Atom	Angle/°
C1-N1-Pt1	128.0(5)	Cl3-Pt2-Cl2	89.54(6)
C5-N1-Pt1	113.4(4)	Cl3^{1}-Pt2-Cl21	89.54(6)
C6-N2-Pt1	118.9(4)	Cl3-Pt2-Cl21	90.46(6)
C10-N2-Pt1	118.6(4)	Cl2-Pt2-Cl21	180.00(9)
C15-N3-Pt1	127.2(5)	Cl3^{1}-Pt2-Cl4	89.61(6)
C11-N3-Pt1	113.7(4)	Cl3-Pt2-Cl4	90.39(6)
N2-Pt1-N1	81.1(2)	Cl2-Pt2-Cl4	90.17(6)
N2-Pt1-N3	81.0(2)	Cl2^{1}-Pt2-Cl4	89.83(6)
N1-Pt1-N3	162.1(2)	Cl3^{1}-Pt2-Cl4^{1}	90.39(6)
N2-Pt1-Cl1	179.26(16)	Cl3-Pt2-Cl4^{1}	89.61(6)
N1-Pt1-Cl1	98.91(17)	Cl2-Pt2-Cl4^{1}	89.83(6)
N3-Pt1-Cl1	99.01(16)	Cl2^{1}-Pt2-Cl4^{1}	90.17(6)
Cl3^{1}-Pt2-Cl3	180.0	Cl4-Pt2-Cl4^{1}	180.00(8)
Cl3^{1}-Pt2-Cl2	90.46(6)		

Table S4 Hydrogen bonding formed by Pt2 with chlorine ions attached to methanol and pyridine on the ligand

H....Acceptor	D - H	H... A	D... A	D - H... A	A..H..A*	A'..H..A"
3O3--H3O..Cl2	0.84	2.48	3.1643(1)	139		
3O3--H3O..Cl3	0.84	2.81	3.4911(1)	139'	76'	354
1C2--H2..O2B	0.95	2.37	3.3015(1)	165		
1C2--H2..O2A	0.95	2.40	3.2970(1)	158'	12'	335
1C7--H7..Cl3	0.95	2.70	3.2637(1)	118		
1C12--H12..Cl3	0.95	2.75	3.5828(1)	146		
1C15--H15..Cl1	0.95	2.73	3.4552(1)	134		
1C18--H18..Cl2	095	2.80	3.5929(1)	141		
1C23--H23B..O2A	0.99	2.58	3.2722(1)	127		
3C28--H28A..Cl3	0.98	2.78	3.4724(1)	128		

Fig. S1 SEM image of CPT-Pt.

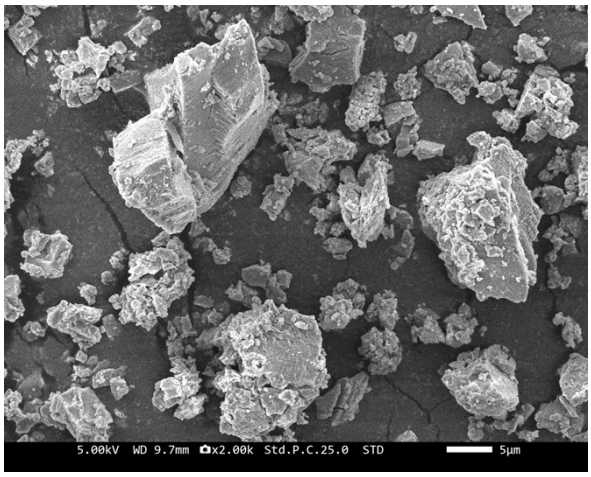

Fig S2 Thermogravimetric diagram of CPT-Pt.

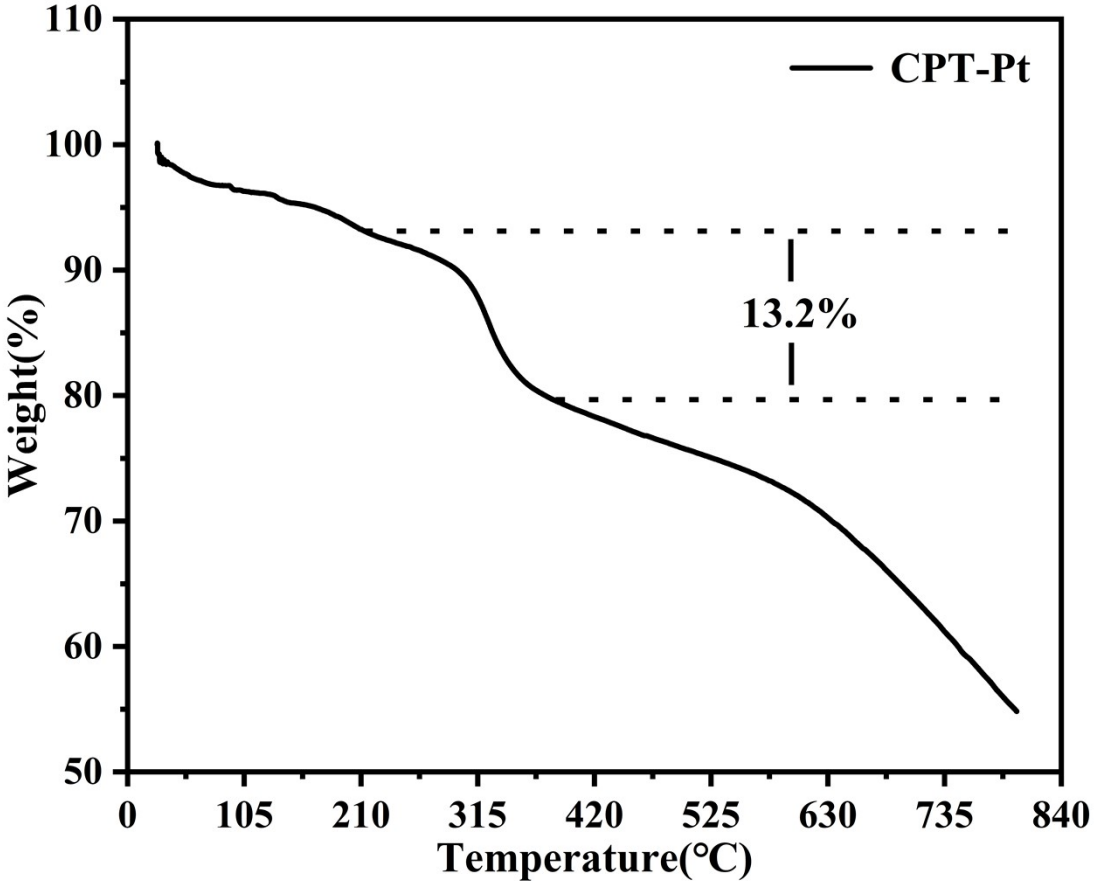

Fig S3 UV absorption spectra of CPT-Pt in water(a) and Tris-buffer (PH=7.4) (b) solution.

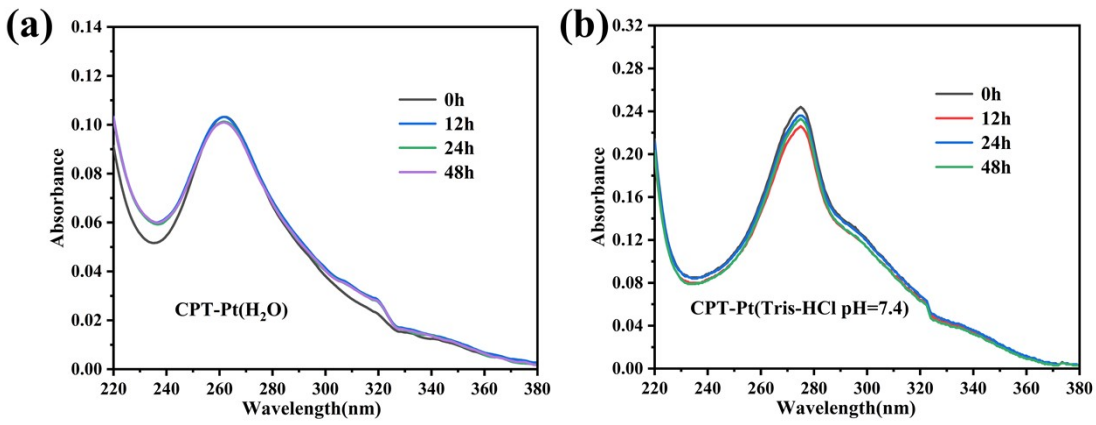

Fig S4 Effect of tested compounds on apoptosis. BxPC-3 cells were exposed to PBS , CPT-Pt (30 μM), oxaliplatin (30 μM).

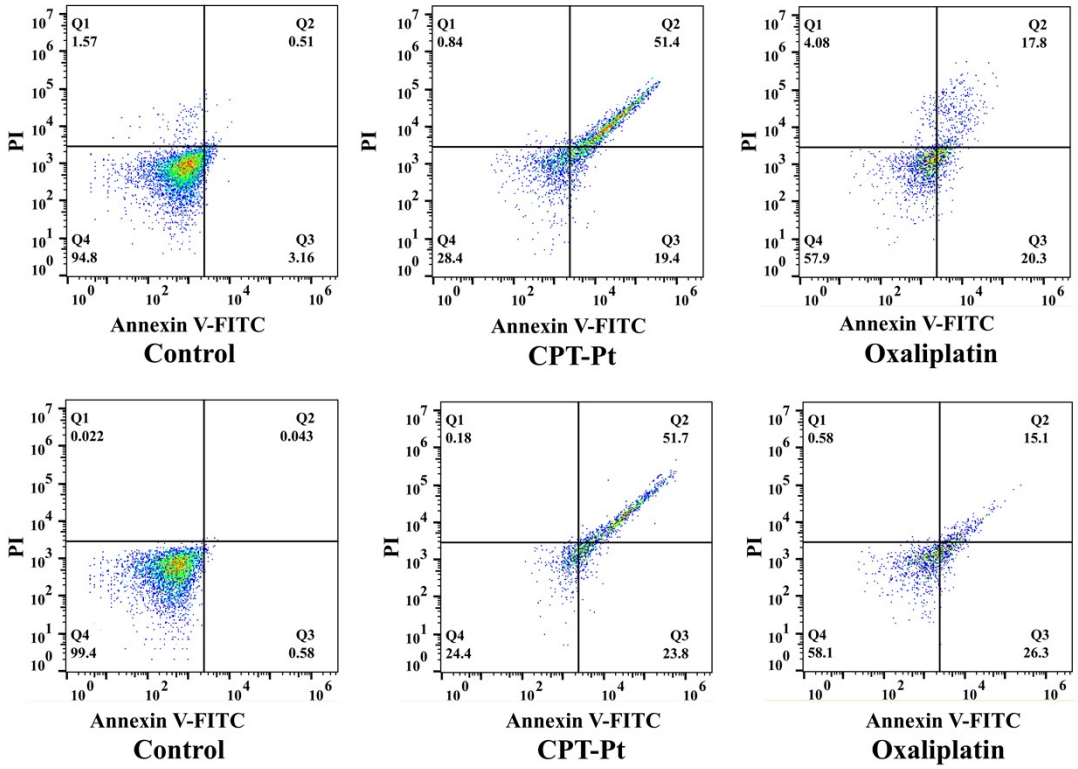

Fig S5 Investigation on CPT-Pt induced cell cycle arrest. BxPC-3 cells were

exposed to PBS (a), CPT-Pt (b, 30 μM), oxaliplatin (c, 30 μM)

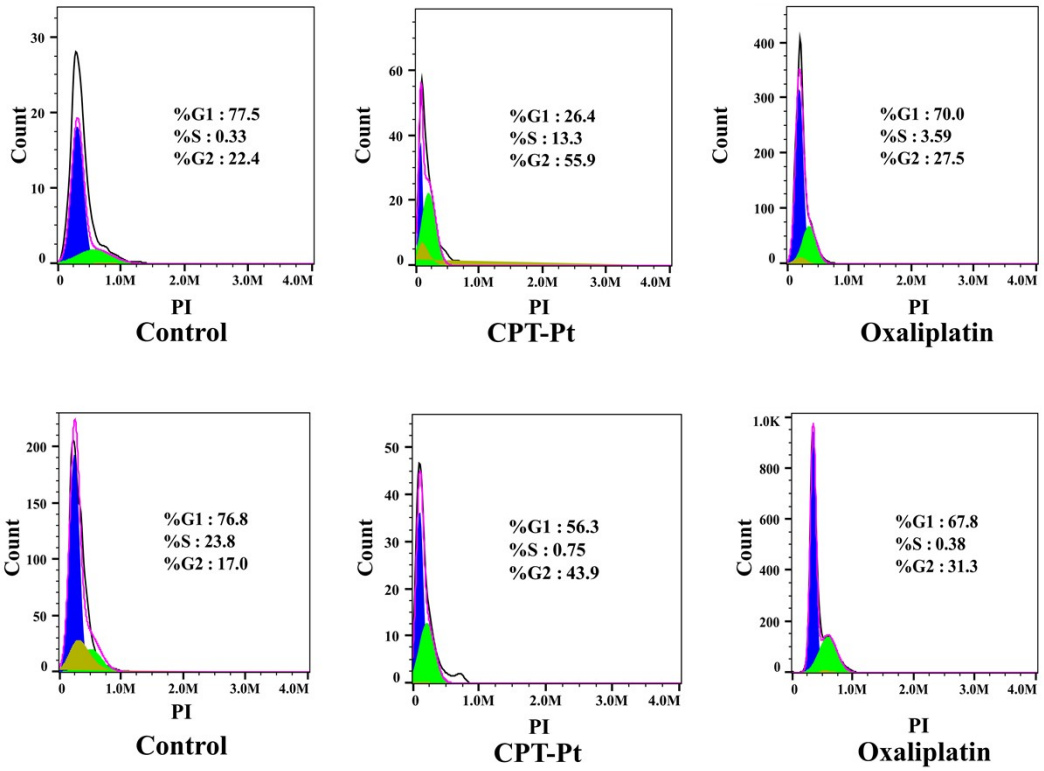

Fig S6 Accumulation of intracellular ROS assay. BxPC-3 cells were treated with PBS, CPT-Pt or Oxaliplatin (10 μM) for 24 h, stained with DCFH-DA and

analyzed via flow cytometry.

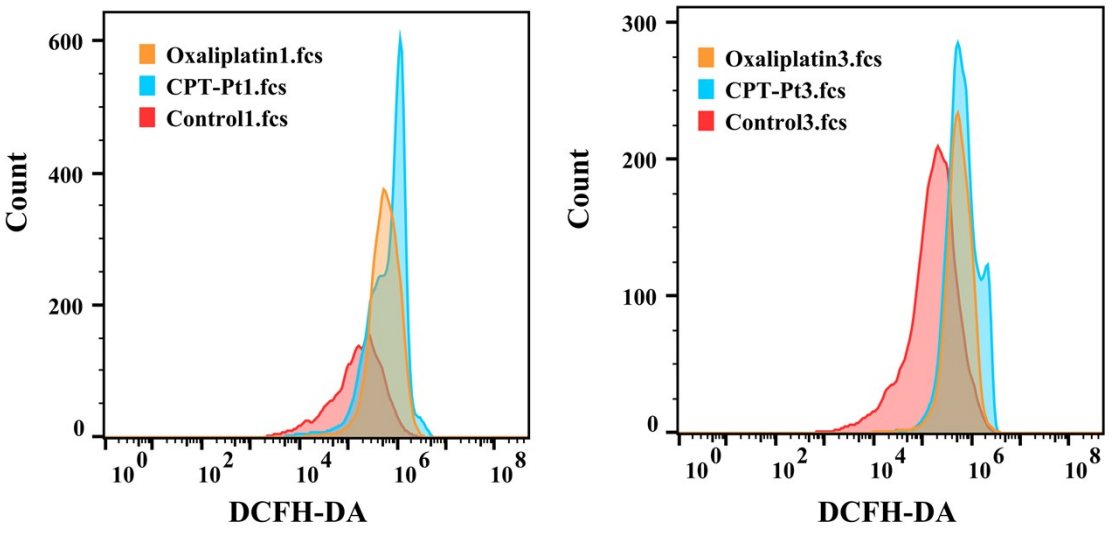

Fig S7 Accumulation of intracellular ROS assay. BxPC-3 cells were treated with PBS, CPT-Pt or Oxaliplatin (30 μM) for 24 h, stained with JC-1 and analyzed via

flow cytometry.