

**A Positively Charged Trinuclear 3N-chelated
Monofunctional Platinum Complex With High DNA Affinity
and Potent Cytotoxicity**

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Crystallographic Data of $[\text{Pt}_3(\text{HPTAB})\text{Cl}_3][\text{PtCl}_3(\text{DMSO})](\text{ClO}_4)_2 \cdot \text{DMSO} \cdot \text{C}_3\text{H}_6\text{O} \cdot \text{CH}_3\text{OH} \cdot \text{H}_2\text{O}$

Experimental section

$[\text{Pt}_3(\text{HPTAB})\text{Cl}_3](\text{ClO}_4)_3$ (**1**)

0.633g of $\text{Pt}(\text{DMSO})_2\text{Cl}_2$ (1.5mmol) was added to a solution of ligand of HPTAB (0.355g, 0.5mmol,) in methanol (15mL). The resulting solution was stirred at room temperature for three days, and then the solids were collected by centrifugation and washed with methanol and diethyl ether. The dried solid redissolved in DMSO containing a few drops of methanol was mixed with saturated NaClO_4 solution of DMSO and a clear solution was obtained. Pale yellow powder was obtained by diffusion of acetone into the solution and identified as complex **1**. Anal. (%) Calcd. for $\text{C}_{45}\text{H}_{45}\text{Cl}_6\text{Pt}_3\text{N}_9\text{O}_{12}$: C, 31.74; H, 2.64; N, 7.40. Found: C, 31.68; H, 2.57; N, 7.56. ES-MS: $m/z = 468.3$ $[\text{Pt}_3(\text{HPTAB})\text{Cl}_3]^{3+}$, 719.8 $[\text{Pt}_3(\text{HPTAB})\text{Cl}_4]^{2+}$, 1474.3 $[\text{Pt}_3(\text{HPTAB})\text{Cl}_5]^+$. $^1\text{H NMR}$ (500MHz, DMSO- d_6 /TMS) δ (ppm) 8.69 (d, 6H,), 8.23 (t, 6H), 7.87 (d,6H), 7.83 (m,3H), 7.61 (t,6H), 5.37 (d,6H), 4.76 (d,6H), 4.19 (m,6H).

Meanwhile, the small amounts of yellow crystals **2** suitable for X-Ray structure analysis were achieved at the same time and mechanically separated from the above pale yellow powder **1**. Structure analysis demonstrated it was quite similar to **1** and possessing the formula of $[\text{Pt}_3(\text{HPTAB})\text{Cl}_3][\text{PtCl}_3(\text{DMSO})](\text{ClO}_4)_2 \cdot \text{DMSO} \cdot \text{C}_3\text{H}_6\text{O} \cdot \text{CH}_3\text{OH} \cdot \text{H}_2\text{O}$. Its ESMS spectrum was identical to that of **1**.

NMR spectra of **L**

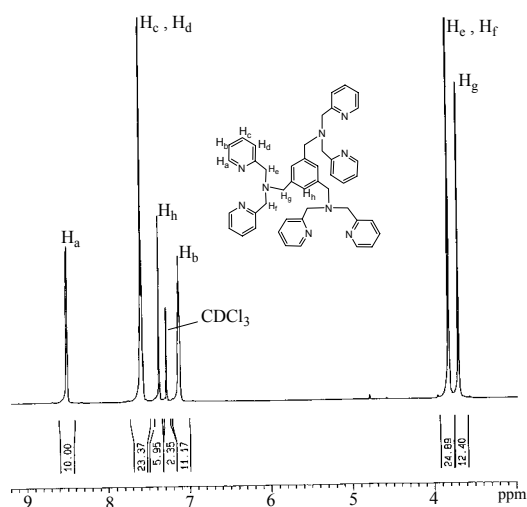


Figure S1. ¹H NMR spectrum of HPTAB in CDCl₃

ESMS Spectra of **1**

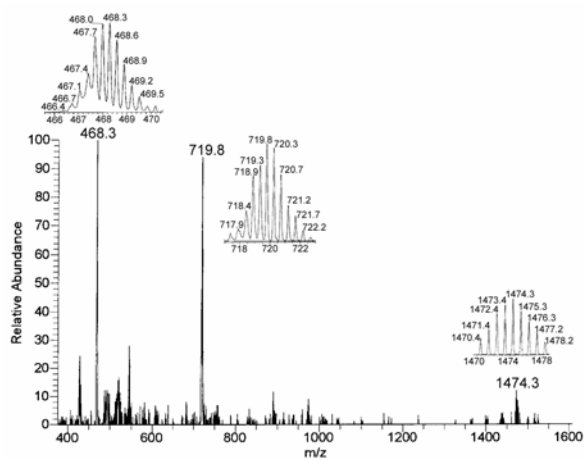


Figure S2. ESMS Spectra of complex **1**; the insets show the isotopic distributions for the main peaks

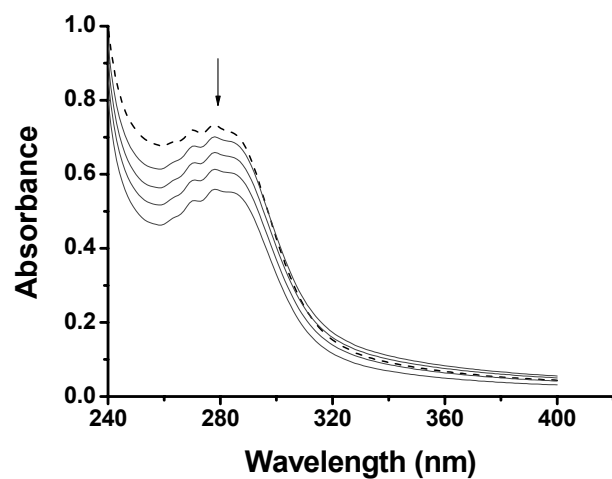


Figure S3. Time dependent absorbance spectra of complex **1** at r ($[DNA]/[complex]$) = 0.5 (—, represent 3,6,9,12h respectively) at room temperature.

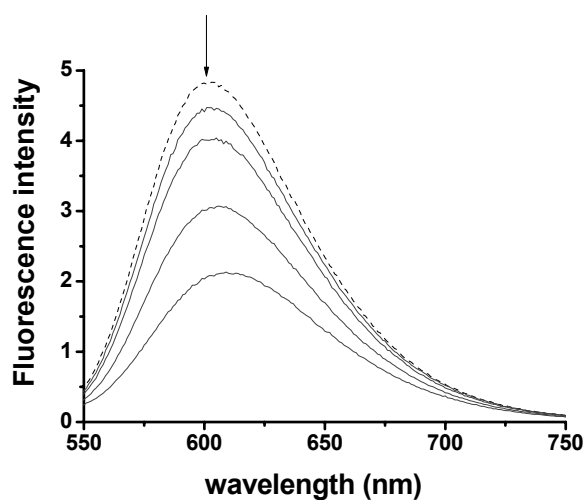


Figure S4. Fluorescence emission spectra (excited at 526 nm) of the EB-DNA system (50 μ M EB, 50 μ M CT-DNA) in the absence (dotted line) and presence (solid line) of **1** (3mM, 10 μ L per scan).

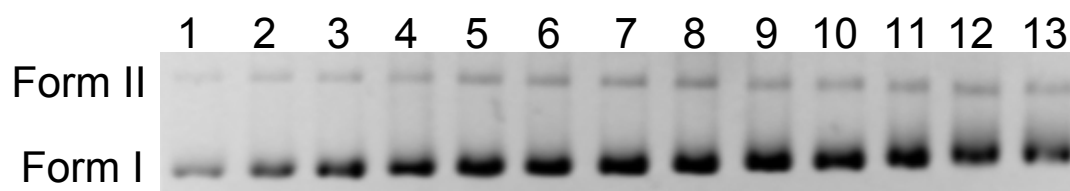


Figure S5. Electrophoresis in agarose gel of pUC19 plasmid DNA incubated for 24h at 37°C with cisplatin. Lane 1, control, Lane 2-13, the r_1 values of 0.015, 0.03, 0.045, 0.06, 0.075, 0.09, 0.12, 0.18, 0.24, 0.30, 0.45, 0.52 respectively.

Crystallographic Data of



Table S1. Selected bond lengths (Å) and angles (°) of [Pt₃(HPTAB)Cl₃][PtCl₃(DMSO)](ClO₄)₂·DMSO·C₃H₆O·CH₃OH·H₂O

Pt1-Cl1	2.291(3)	Pt1-N1	1.999(8)	Pt1-N2	2.025(10)
Pt1-N3	2.021(10)	Pt2-Cl2	2.289(2)	Pt2-N4	1.987(9)
Pt2-N5	2.028(9)	Pt2-N6	1.962(9)	Pt3-Cl3	2.283(2)
Pt3-N7	2.027(8)	Pt3-N8	1.986(8)	Pt3-N9	2.001(8)
Cl1-Pt1-N1	177.9(2)	N2-Pt1-N3	167.6(4)	Cl2-Pt2-N4	176.4(2)
N5-Pt2-N6	167.9(4)	Cl3-Pt3-N7	178.0(2)	N8-Pt3-N9	166.7(3)