

Supplementary Material

A novel star-shaped trinuclear platinum(II) complex based on a 1,3,5-triazine core displaying potent antiproliferative activity against TNBC by mitochondria injury and DNA damage mechanism

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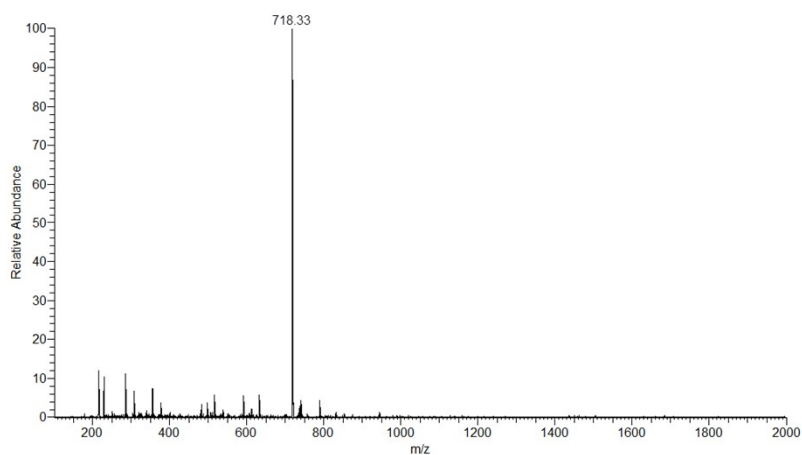


Fig. S1 ESI-MS spectra of 2,4,6-tris[(2-hydroxybenzyl)(2-pyridylmethyl)amine]-1,3,5-triazine (**L**) in methanol.

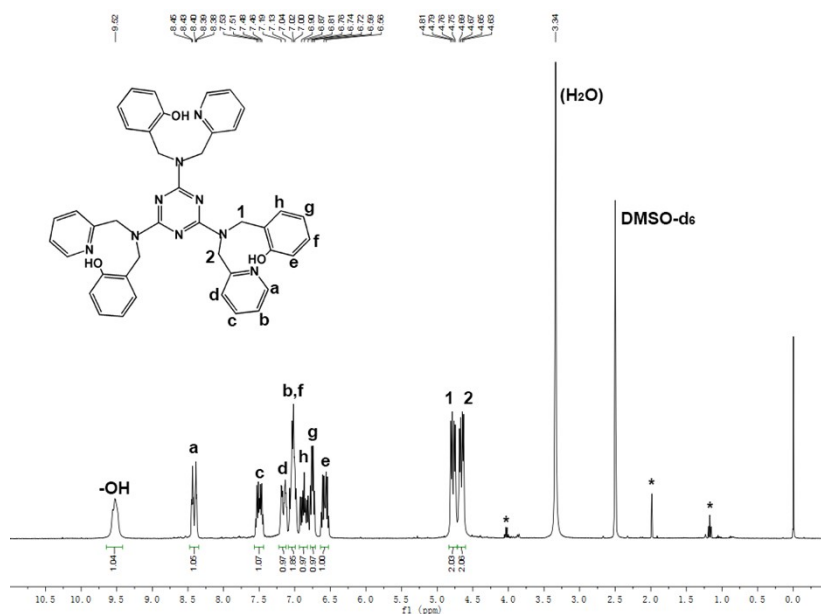


Fig. S2 ¹H NMR of 2,4,6-tris[(2-hydroxybenzyl)(2-pyridylmethyl)amine]-1,3,5-triazine (**L**) in DMSO-*d*₆. The signals marked with * are for the protons from residual solvent ethyl acetate.

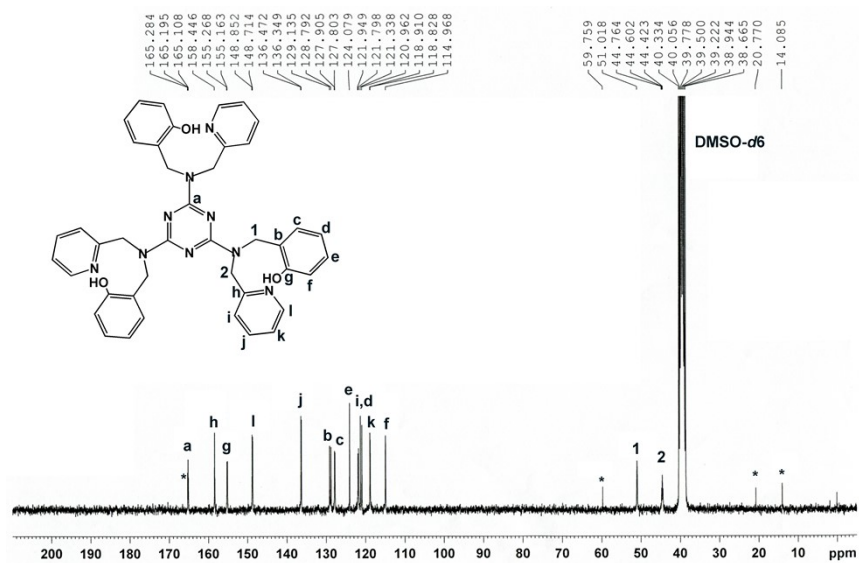


Fig. S3 ^{13}C NMR of 2,4,6-tris[(2-hydroxybenzyl)(2-pyridylmethyl)amine]-1,3,5-triazine (**L**) in $\text{DMSO-}d_6$. The signals marked with * are for the carbons from residual solvent ethyl acetate.

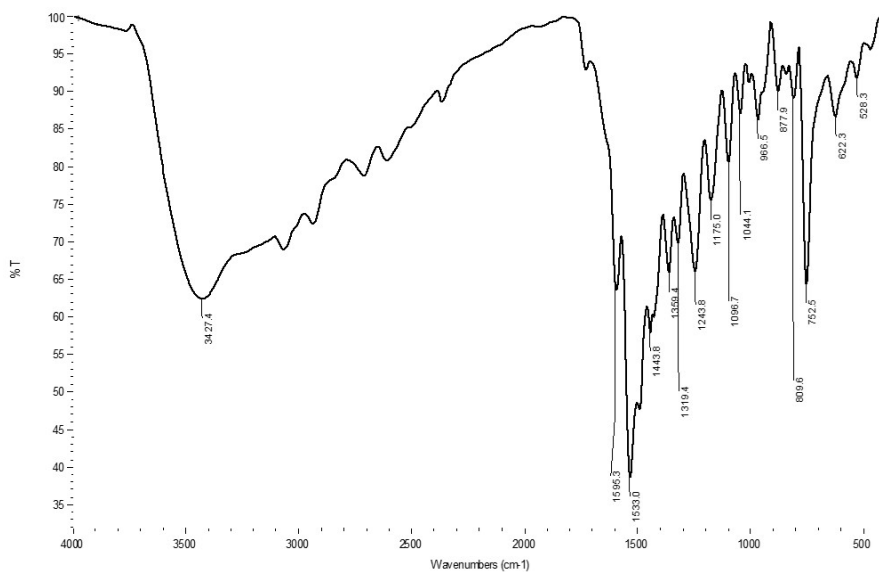


Fig. S4 IR Spectra of 2,4,6-tris[(2-hydroxybenzyl)(2-pyridylmethyl)amine]-1,3,5-triazine (**L**).

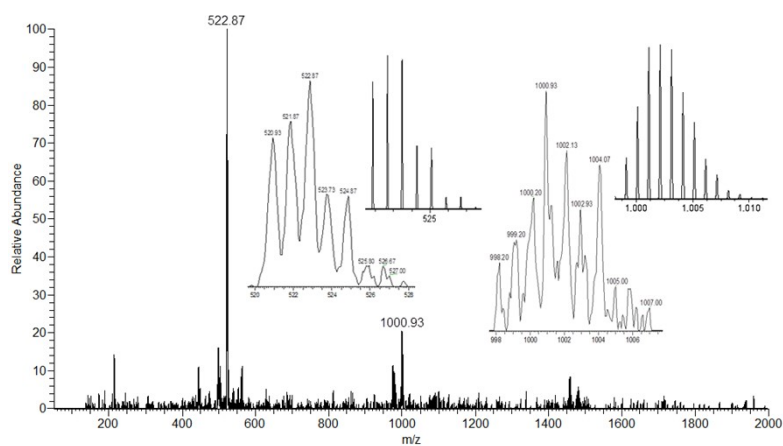


Fig. S7 ESI-MS spectra of complex **2** in methanol.

Table S1 Characteristic IR bands (cm^{-1}) of the ligands and their respective platinum(II) complexes.

Assignment	$[\text{Pt}_3(\text{L}-3\text{H})\text{Cl}_3]$ (1)	L	$[\text{Pt}(\text{L}'-\text{H})\text{Cl}]$ (2)	L'
$\nu_{\text{C-H}}$ aromatic	3088	3032	3147	3049
$\nu_{\text{C=N}}$	1533	1533	1603	1593
$\nu_{\text{C=C}}$	1485	1443	1452	1457
$\delta(\text{pyridine ring})$	761	752	766	752
$\delta(\text{OH-phenol})$	—	1359	—	1351

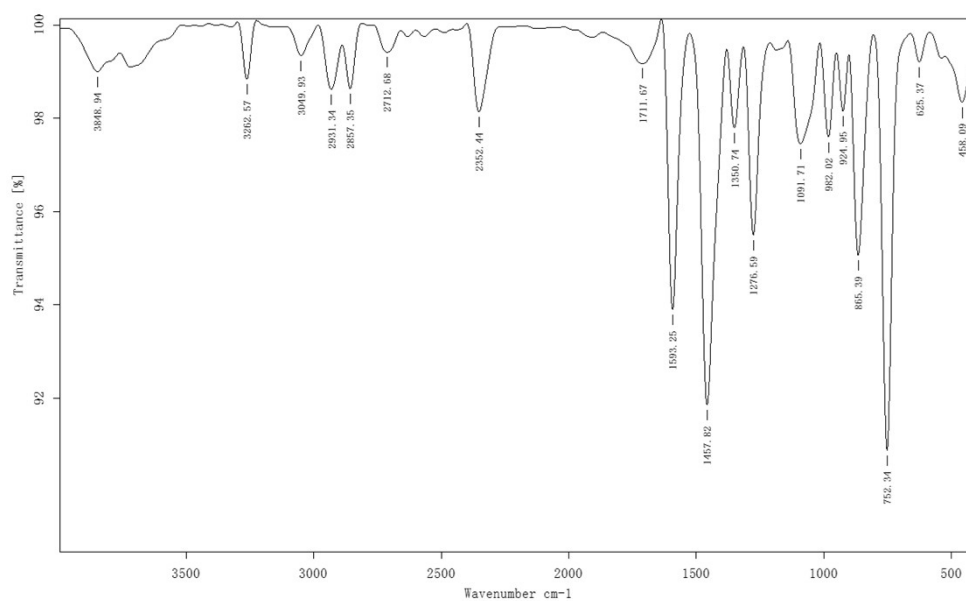


Fig. S8 IR Spectra of (2-hydroxybenzyl)(2-pyridylmethyl)amine (**L'**).

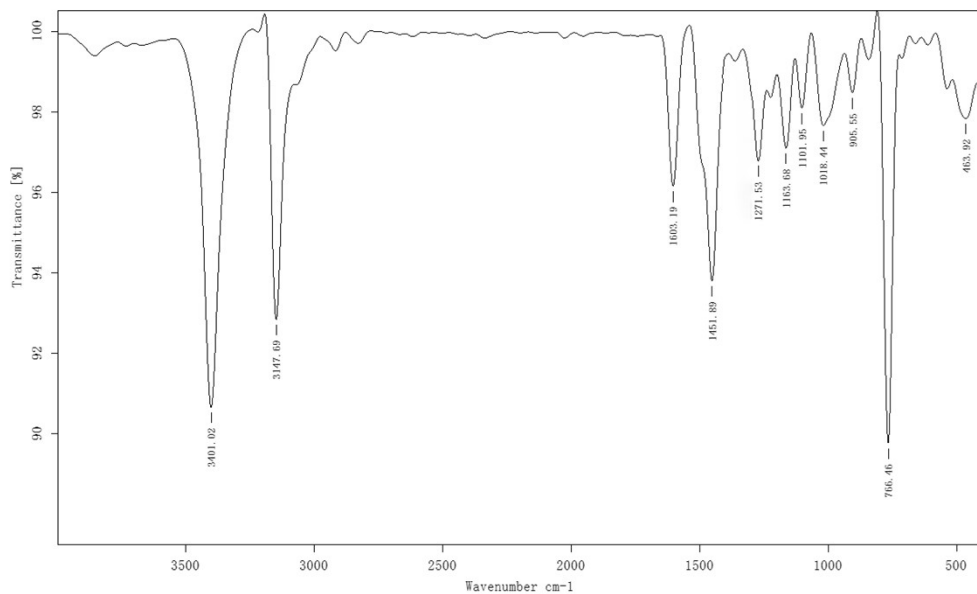


Fig. S9 IR Spectra of complex 2.

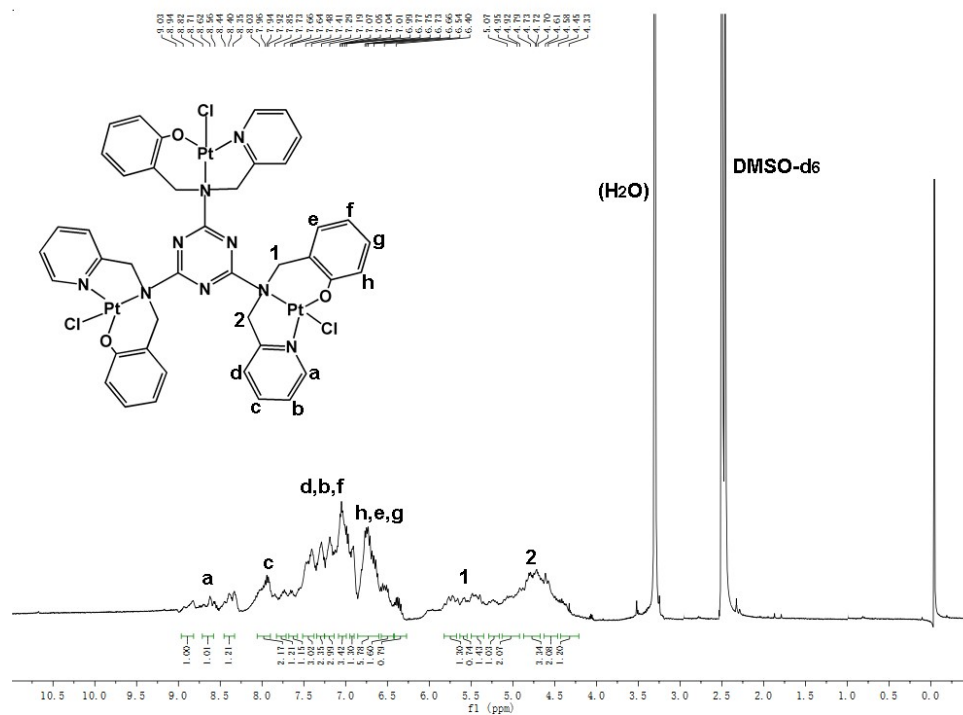


Fig. S10 ^1H NMR spectra of $[\text{Pt}_3(\text{L}-3\text{H})\text{Cl}_3]$ (1) in $\text{DMSO}-d_6$.

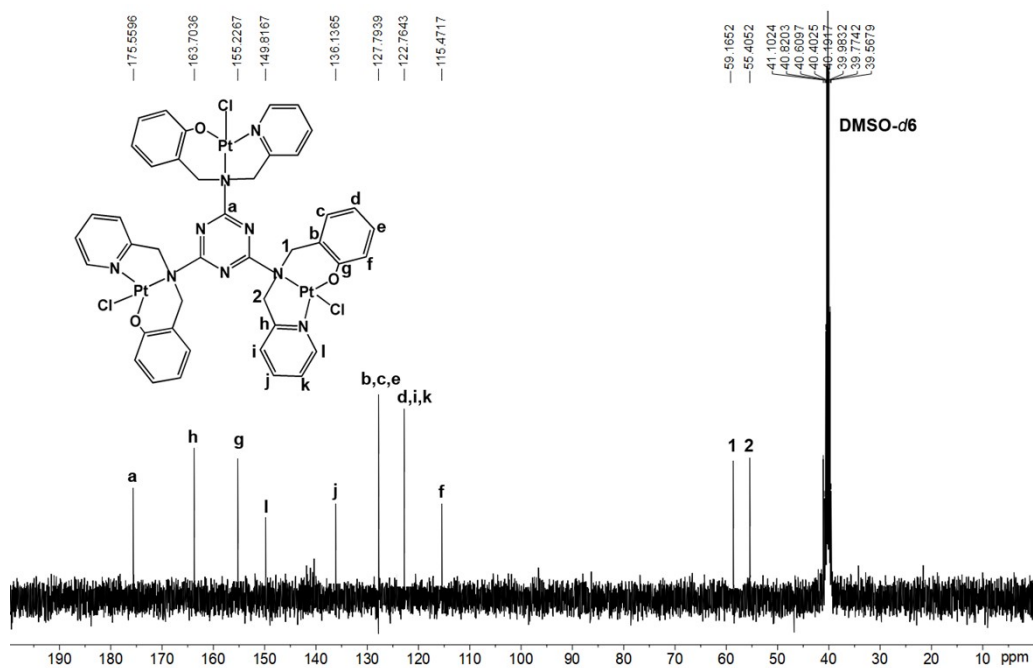


Fig. S11 ^{13}C NMR spectra of $[Pt_3(L-3H)Cl_3]$ (1) in DMSO- d_6 .

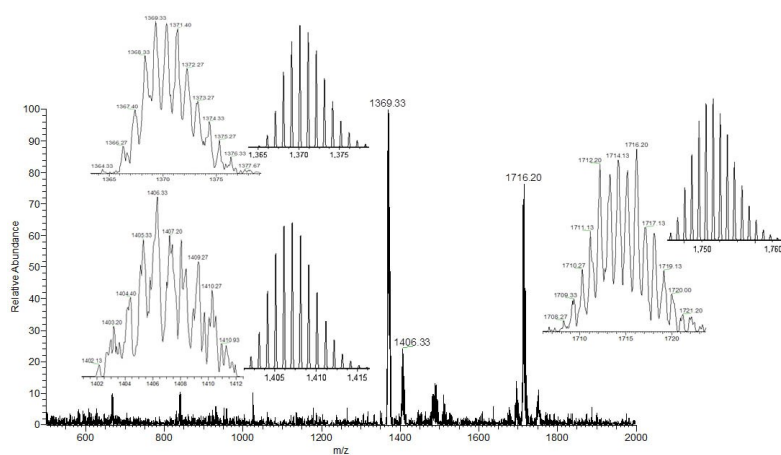


Fig. S12 ESI-MS spectra of complex 1 in methanol.

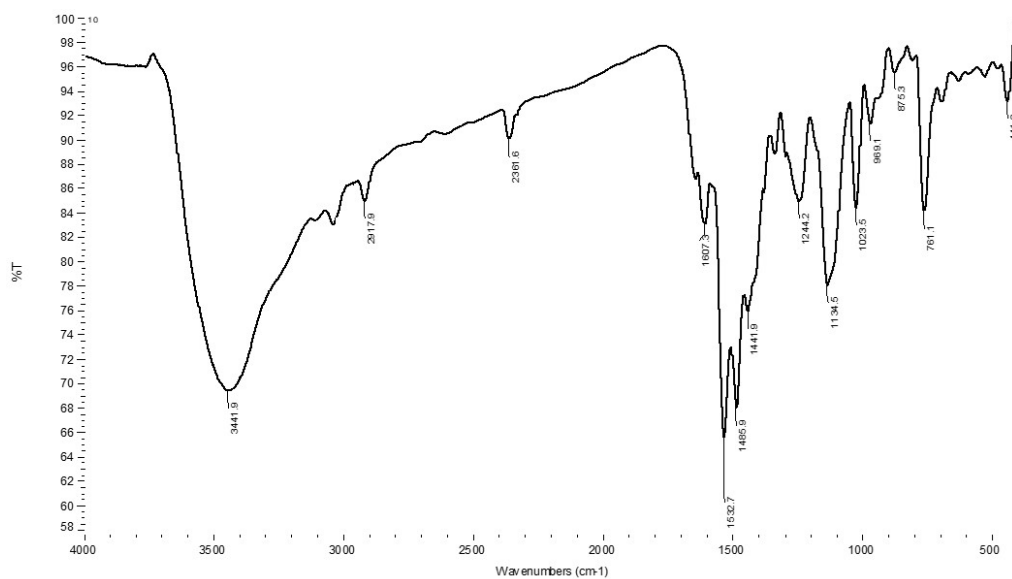


Fig. S13 IR Spectra of complex 1.

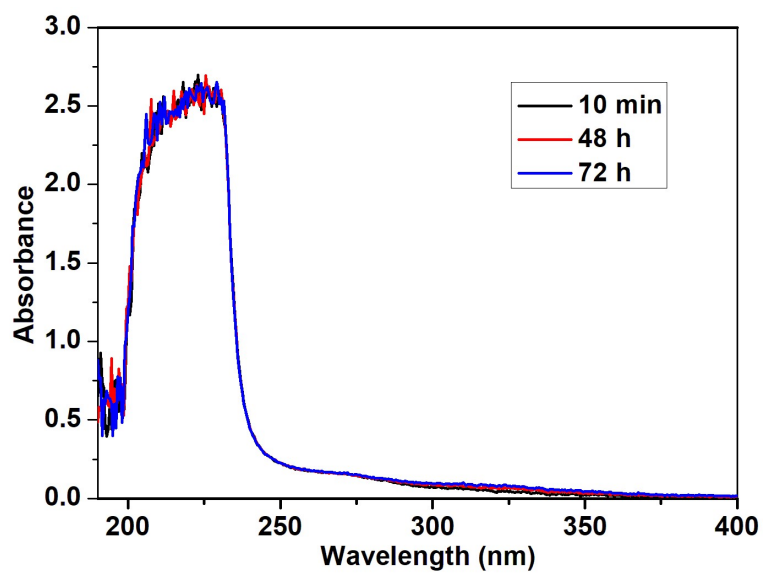


Fig. S14 The absorption spectra of 1 (25 μ M, 0.3% DMSO) in cell culture media (Roswell Park Memorial Institute (RPMI) 1640 medium) at 10 min, 48 h, 72 h.

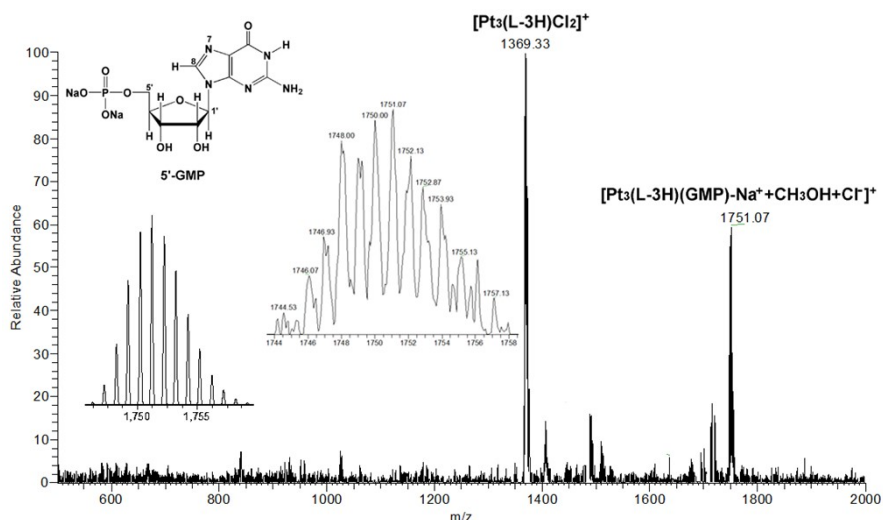


Fig. S15 ESI-MS spectrum (positive mode) of the reaction between complex **1** and 5'-GMP (1: 3.5) recorded in methanol/water (v/v, 1:1) at 37 °C for 24 h. Assignments: 1751.07, $[\text{Pt}_3(\text{L}-3\text{H})(\text{GMP})-\text{Na}^+ + \text{CH}_3\text{OH} + \text{Cl}]^+$ ($\text{Pt}_3\text{C}_{53}\text{H}_{52}\text{N}_{14}\text{O}_{12}\text{PNaCl}$, calcd 1751.31); 1369.33, $[\text{Pt}_3(\text{L}-3\text{H})\text{Cl}_2]^+$ ($\text{Pt}_3\text{C}_{42}\text{H}_{36}\text{N}_9\text{O}_3\text{Cl}_2$, calcd 1369.12).

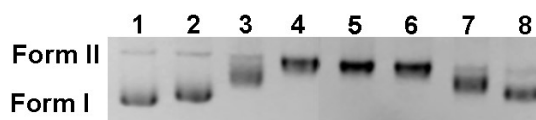


Fig. S16 Agarose gel electrophoresis patterns of supercoiled pUC19 plasmid DNA incubated with complex **1** at 37 °C for 24 h. Lane 1, control; lanes 2–8, the r_1 values of 0.015, 0.03, 0.045, 0.06, 0.12, 0.18, 0.24, respectively.