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

Yixuan Wu, Dandan Zhao, Jinting Shang, Wenxin Huang, Zhanfen Chen*

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

Fig. S2 $^1$H 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 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. S5 $^1$H NMR of complex 2 in DMSO-$d_6$. The signals marked with * are for the protons from residual solvent diethyl ether.

Fig. S6 $^1$H NMR of (2-hydroxybenzyl)(2-pyridylmethyl)amine ($L'$) in DMSO-$d_6$. The signals marked with * are for the protons from residual solvent diethyl ether.
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.

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

Fig. S8 IR Spectra of (2-hydroxybenzyl)(2-pyridylmethyl)amine (L$'$).
Fig. S9 IR Spectra of complex 2.

Fig. S10 $^1$H NMR spectra of [Pt$_3$(L–3H)Cl$_3$] (1) in 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 μM, 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, \([\text{Pt}_3(\text{L}^{-3H})(\text{GMP})-\text{Na}+\text{CH}_3\text{OH}+\text{Cl}]^+\) (Pt$_3$C$_{53}$H$_{52}$N$_{14}$O$_{12}$PNaCl, calcd 1751.31); 1369.33, \([\text{Pt}_3(\text{L}^{-3H})\text{Cl}_2]^+\) (Pt$_3$C$_{42}$H$_{36}$N$_9$O$_3$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.