Enhancement of therapeutic effect in breast cancer with a steroid-conjugated ruthenium complex

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Figure S1 The synthesis procedure of Te-S-S-NHC-Ru.

Figure S2 The ESI-MS of compound Pr-OH.

Figure S3 The ESI-MS of compound Pr-S-S-NHC.
Figure S4 The ESI-MS of compound Te-S-S-NHC-Ru.

Figure S5 The $^1$H/NMR spectrum of compound Te-S-S-NHC-Ru. (arrow point: four hydrogen atoms were covered by water signal.)
Figure S6 The $^{13}$C/NMR spectrum of compound Te-S-S-NHC-Ru.

Figure S7 The stability of compound Te-S-S-NHC-Ru in PBS (pH 7.4) at 12 h and 24 h.

Figure S8 The HPLC chromatogram of compound Te-S-S-NHC-Ru in various amino acids and metal salts solutions (5 mM) stirring at 37 °C for 60 min.
Table S1: IC₅₀ values of complexes NHC-Ru, Te-S-S-NHC-Ru and cisplatin against MCF-7, MDA-MB-231 and LO2 cell lines.

<table>
<thead>
<tr>
<th>Complexes</th>
<th>MCF-7 (μM)</th>
<th>MDA-MB-231 (μM)</th>
<th>Hs 578Bst (μM)</th>
</tr>
</thead>
<tbody>
<tr>
<td>NHC-Ru</td>
<td>10.54±0.34</td>
<td>14.18±1.01</td>
<td>11.42±1.12</td>
</tr>
<tr>
<td>Te-S-S-NHC-Ru</td>
<td>4.48±0.17</td>
<td>20.71±0.92</td>
<td>37.36±1.89</td>
</tr>
<tr>
<td>Cisplatin</td>
<td>24.94±2.66</td>
<td>30.0±1.62</td>
<td>26.58±2.64</td>
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</tbody>
</table>

*Inhibitory activity was assayed by exposure of cell lines to the complex for 48 h and expressed as a concentration required to inhibit the cell proliferation by 50% (IC₅₀). Data were expressed as the means ± SD of three independent experiments.

**Figure S9.** Cell cycle distribution of MCF-7 and MBA-MD-231 cancer cells treated with Te-S-S-NHC-Ru (5, 10, and 15 μM) for 48 h.
**Figure S10.** Biodistribution of Ru in main organs after two weeks treatment of NHC-Ru and Te-S-S-NHC-Ru in MCF-7 xenografts nude mice by using ICP-MS.