## Electronic Supplementary Material (ESI) for New Journal of Chemistry

## 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 <sup>1</sup>H/NMR spectrum of compound Te-S-S-NHC-Ru. (arrow point: four hydrogen atoms were covered by water signal.)



Figure S6 The <sup>13</sup>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 ℃ for 60 min.

Complexes -	$IC_{50}(\mu M)^{a}$		
	MCF-7	MDA-MB-231	Hs 578Bst
NHC-Ru	10.54±0.34	14.18±1.01	11.42±1.12
Te-S-S-NHC-Ru	4.48±0.17	20.71±0.92	37.36±1.89
Cisplatin	24.94±2.66	30.0±1.62	26.58±2.64

**Table S1** IC<sub>50</sub> values of complexes NHC-Ru, Te-S-S-NHC-Ru and cisplatin against MCF-7, MDA-MB-231 and LO2 cell lines.

<sup>a</sup>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% (IC<sub>50</sub>). Data were expressed as the means  $\pm$  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  $\mu$ M) 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.