Supporting Information for

Synthesis, characterization, photoluminescence, anti-tumor activity, DFT calculations and molecular docking with proteins of zinc (II) halogen substituted terpyridine compounds

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Fig. S1 The $^1$H NMR spectrum of compound 1.

Fig. S2 The $^1$H NMR spectrum of compound 2.
Fig. S3 The $^1$H NMR spectrum of compound 4.

Fig. S4 The $^1$H NMR spectrum of compound 5.
Fig. S5 The $^1$H NMR spectrum of compound 6.

Fig. S6 The $^1$H NMR spectrum of compound 7.
Fig. S7 The $^1$H NMR spectrum of compound 8.

Fig. S8 The IR spectrum of compound 1.
Fig. S9 The IR spectrum of compound 2.

Fig. S10 The IR spectrum of compound 4.

Fig. S11 The IR spectrum of compound 5.
Fig. S12 The IR spectrum of compound 6.

Fig. S13 The IR spectrum of compound 7.

Fig. S14 The IR spectrum of compound 8.
**Fig. S15.** UV–vis spectra of compounds 2 for a period of 24 h.

**Fig. S16.** UV–vis spectra of compounds 3 for a period of 24 h.
**Fig.S17.** UV–vis spectra of compounds 4 for a period of 24 h.

**Fig.S18.** UV–vis spectra of compounds 5 for a period of 24 h.

**Fig.S19.** UV–vis spectra of compounds 6 for a period of 24 h.
Fig. S20. UV–vis spectra of compounds 8 for a period of 24 h.

Fig. S21. The standard curves of UV–vis spectra for compounds 1-8.
<table>
<thead>
<tr>
<th>Compound concentration</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
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<tr>
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<td>0.5μM</td>
<td>0.3μM</td>
<td>0.1μM</td>
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<tr>
<td>C1</td>
<td>2.8μM</td>
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<td>2.8μM</td>
<td>0.7μM</td>
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<tr>
<td>C2</td>
<td>11.4μM</td>
<td>17.0μM</td>
<td>11.4μM</td>
<td>3.0μM</td>
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<th>6</th>
<th>7</th>
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<tr>
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<td>0.2μM</td>
<td>0.2μM</td>
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<tr>
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<tr>
<td>C2</td>
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<td>2.8μM</td>
<td>6.8μM</td>
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Fig. S22 The morphology of A549 cells treated with cisplatin (C1: 2.6 μM and C2: 43 μM) or compounds 1-8 with series concentrations (the numbers in the pictures indicate the concentration of the compounds with the unit of μM). The control inset shows the cell morphology without any complexes.
**Fig. S23** The morphology of Bel-7049 cells treated with cisplatin (C1: 2.6 μm and C2: 43 μM) or compounds 1-8 with series concentrations (the numbers in the pictures indicate the concentration of the compounds with the unit of μM). The control inset shows the cell morphology without any complexes.
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<td>0.2μM</td>
</tr>
<tr>
<td>C1</td>
<td>1.4μM</td>
<td>0.7μM</td>
<td>1.7μM</td>
<td>1.5μM</td>
</tr>
<tr>
<td>C2</td>
<td>5.7μM</td>
<td>3.0μM</td>
<td>6.8μM</td>
<td>5.9μM</td>
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</table>

**Fig. S24** The morphology of MCF-7 cells treated with cisplatin (C1: 2.6 μm and C2: 43 μM) or compounds 1-8 with series concentrations (the numbers in the pictures indicate the concentration of the compounds with the unit of μM). The control inset shows the cell morphology without any complexes.
**Fig.S25.** Fluorescence emission spectra of compound 2 with or without ctDNA. The added ctDNA concentrations were 0, 1.06, 2.12, 3.18, 4.24, 5.30, 6.36, 7.42, 8.48 μM. The inset shows the curves of F₀/F vs. [Q] of compound 2 (R is the correlated coefficient for the Ksv values).

**Fig.S26.** Fluorescence emission spectra of compound 3 with or without ctDNA. The added ctDNA concentrations were 0, 1.06, 2.12, 3.18, 4.24, 5.30, 6.36, 7.42, 8.48 μM. The inset shows the curves of F₀/F vs. [Q] of compound 3 (R is the correlated coefficient for the Ksv values).
**Fig. S27.** Fluorescence emission spectra of compound 4 with or without ctDNA. The added ctDNA concentrations were 0, 1.06, 2.12, 3.18, 4.24, 5.30, 6.36, 7.42, 8.48 μM. The inset shows the curves of $F_0/F$ vs. [Q] of compound 4 (R is the correlated coefficient for the $K_{sv}$ values).

**Fig. S28.** Fluorescence emission spectra of compound 5 with or without ctDNA. The added ctDNA concentrations were 0, 1.06, 2.12, 3.18, 4.24, 5.30, 6.36, 7.42, 8.48 μM. The inset shows the curves of $F_0/F$ vs. [Q] of compound 5 (R is the correlated coefficient for the $K_{sv}$ values).
**Fig. S29.** Fluorescence spectra of compound 6 with or without ctDNA. The added ctDNA concentrations were 0, 1.06, 2.12, 3.18, 4.24, 5.30, 6.36, 7.42, 8.48 μM. The inset shows the curves of $F_0/F$ vs. [Q] of compound 6 (R is the correlated coefficient for the $K_m$ values).

**Fig. S30.** Fluorescence spectra of compound 8 with or without ctDNA. The added ctDNA concentrations were 0, 1.06, 2.12, 3.18, 4.24, 5.30, 6.36, 7.42, 8.48 μM.
**Fig. S31** CD spectrum of ctDNA in the presence of complexes 2.

**Fig. S32** CD spectrum of ctDNA in the presence of complexes 3.

**Fig. S33** CD spectrum of ctDNA in the presence of complexes 4.
Fig.S34 CD spectrum of ctDNA in the presence of complexes 5.

Fig.S35 CD spectrum of ctDNA in the presence of complexes 6.

Fig.S36 CD spectrum of ctDNA in the presence of complexes 8.
Fig. S37 2D and 3D binding modes of compound 2 with HSP90 (A), ALK kinase domain (B), EGFR kinase domain (C) and HER2 kinase domain (D).
Fig. S38 2D and 3D binding modes of compound 3 with HSP90 (A), ALK kinase domain (B), EGFR kinase domain (C) and HER2 kinase domain (D).
**Fig. S39** 2D and 3D binding modes of compound 4 with HSP90 (A), ALK kinase domain (B), EGFR kinase domain (C) and HER2 kinase domain (D).
Fig. S40 2D and 3D binding modes of compound 5 with HSP90 (A), ALK kinase domain (B), EGFR kinase domain (C) and HER2 kinase domain (D).
Fig. S41 2D and 3D binding modes of compound 6 with HSP90 (A), ALK kinase domain (B), EGFR kinase domain (C) and HER2 kinase domain (D).
Fig. S42 2D and 3D binding modes of compound 7 with HSP90 (A), ALK kinase domain (B), EGFR kinase domain (C) and HER2 kinase domain (D).
Fig. S43 2D and 3D binding modes of compound 8 with HSP90 (A), ALK kinase domain (B), EGFR kinase domain (C) and HER2 kinase domain (D).