Supporting information for Submission to Dalton Trans.

Double-strand DNA cleavage by copper complexes of 2,2’-dipyridyl with guanidinium/ammonium pendants

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**Fig. S5**  Agarose gel showing cleavage of 38 μM pBR322 DNA incubated with 150 μM of compounds in 20 mM HEPES buffer, pH 7.2 at 37 °C for 1h. Lane C: DNA control, Lane 1: DNA + L1, Lane 2: DNA + L2, Lane 3: DNA + Cu(ClO₄)₂, Lane 4: DNA + 1, Lane 5: DNA + 2.

**Fig. S6**  Agarose gel showing cleavage of 38 μM pBR322 DNA incubated with 150 μM of complex in 20 mM HEPES buffer, pH 7.2 at 37 °C for 1h for 1 and 2. Lane C: DNA control, Lane 1: DNA + 1, Lanes 2-4: DNA + 1 +100U/mL, 500U/mL, 1,000U/mL Catalase, Lane 5: DNA + 2, Lanes 6-8: DNA + 2 +100U/mL, 500U/mL, 1,000U/mL Catalase.

**Fig. S7**  Kinetics for the cleavage of plasmid pBR322 DNA by 3 (150, 300, 500, 1000 μM) in 20 mM HEPES buffer, pH 7.2 at 37 °C. The samples were run on a 0.9 % agarose gel and stained with ethidium bromide.

**Fig. S8**  Agarose gel showing cleavage of 38 μM pBR322 DNA incubated with 150 μM of complex in 20 mM buffer (MES, MOPSO, TRIS, CHES or CAPS according to pH) at 37 °C for 1 after 0.5h incubation.

**Fig. S9**  Titration condition: 50 mM Tris-HCl ( 50 Mm NaClO₄ ) at pH 7.2, [complex]=25 μM, initial [NaCl] = 200 mM, drop 1 μL NaCl solution to the buffer each time (it means that the concentration of NaCl increase 50 μM).
Figure S1 $^1$H NMR spectrum of L$^1$.

Fig. S2 ESI-MS spectrum of L$^1$
Fig. S3  $T_m$ curves of 100 μM CT DNA in 20 mM pH 8.0 HEPES buffer, 0.1 M NaClO$_4$, in each graph containing no Cu complex(■), 10 μM of 1 (a), 2 (b) and 3 (c) (●), 20 μM of 1 (a), 2 (b) and 3 (c) (▲).
**Fig. S4** Agarose gel electrophoresis (a) and corresponding time course plots (b) showing cleavage of pBR322 DNA by complex 1 and 2 (60-300 μM) in 20 mM pH 7.2 HEPES buffer at 37 °C. In plans, lane C means DNA control, in graphs, symbol ■ indicates the experimental data for the SC forms. The lines connecting them are single exponential fits.

**Table S1** $k_{obs}$ for the cleavage of pBR322 DNA by different concentrations of complexes.

<table>
<thead>
<tr>
<th>Concentration of complex / μM</th>
<th>$k_{obs}$ of 1 / h⁻¹ (R²)</th>
<th>$k_{obs}$ of 2 / h⁻¹ (R²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>60</td>
<td>1.91 (0.876)</td>
<td>1.49 (0.992)</td>
</tr>
<tr>
<td>90</td>
<td>2.37 (0.989)</td>
<td>1.86 (0.981)</td>
</tr>
<tr>
<td>120</td>
<td>2.73 (0.963)</td>
<td>2.24 (0.968)</td>
</tr>
<tr>
<td>150</td>
<td>3.06 (0.997)</td>
<td>2.53 (0.994)</td>
</tr>
<tr>
<td>180</td>
<td>3.21 (0.972)</td>
<td>2.60 (0.935)</td>
</tr>
<tr>
<td>210</td>
<td>3.32 (0.925)</td>
<td>2.81 (0.956)</td>
</tr>
<tr>
<td>300</td>
<td>3.41 (0.996)</td>
<td>3.07 (0.977)</td>
</tr>
</tbody>
</table>

**Fig. S5** Agarose gel showing cleavage of 38 μM pBR322 DNA incubated with 150 μM of compounds in 20 mM HEPES buffer, pH 7.2 at 37 °C for 1h. Lane C: DNA control, Lane 1: DNA + L¹, Lane 2: DNA + L², Lane 3: DNA + Cu(ClO₄)₂, Lane 4: DNA + 1, Lane 5: DNA + 2.
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**Fig. S8**  Agarose gel showing cleavage of 38 μM pBR322 DNA incubated with 150 μM of 1 in 20 mM buffer (MES, MOPS, TRIS, CHES or CAPS according to pH) at 37 °C after 0.5h incubation.

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