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Supplementary Material

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Mixed ligand ruthenium(II) complexes of bis(pyrid-2-yl)-/bis(benzimidazol-2-yl)-dithioether and diimines: Study of non-covalent DNA binding and cytotoxicity

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^{1}H NMR (DMSO-d$_6$, 400 MHz)

The chemical shifts of the free and coordinated ligands (Scheme 1) are given below, along with the coordination-induced shifts (c.i.s. = $\delta_{complex}$ - δ_{ligand}) and coupling constants. Spectral assignments were made on the basis of COSY spectra of the complexes and the J values are consistent with the assignment.

pdto : δ (multiplicity, integration, assignment), ppm 8.487 (d, 2H, H_a), 7.209 (t, 2H, H_b), 7.687 (t, 2H, H_c), 7.301 (d, 2H, H_d), 3.367 (t, 4H, H_e), 2.974 (m, 4H, H_f), 2.922 (t, 4H, H_g).

bbdo : δ (multiplicity, integration, assignment), ppm 7.472 (dd, 2H, H_a), 7.115 (dd, 2H, H_b), 7.115 (dd, 2H, H_c), 7.472 (dd, 2H, H_d), 3.086 (t, 4H, H_e), 3.003 (t, 4H, H_f), 2.749 (s, 4H, H_g).

phen : δ (multiplicity, integration, assignment), ppm 8.570 (dd, 2H, H_2), 7.864 (q, 2H, H_3), 9.248 (dd, 2H, H_4), 8.048 (s, 2H, H_5).

dpq : δ (multiplicity, integration, assignment), ppm 9.221 (d, 2H, H_2), 7.923 (dd, 2H, H_3), 9.432 (d, 2H, H_4), 9.134 (s, 2H, H_7).

dppz : δ (multiplicity, integration, assignment), ppm 9.182 (d, 2H, H_2), 7.905 (t, 2H, H_3), 9.457 (d, 2H, H_4), 8.329 (d, 2H, H_8), 8.030 (t, 2H, H_9).

[Ru(pdto)(phen)](ClO_4)$_2$ 1 : δ (multiplicity, integration, assignment, J/Hz, coordination-induced shifts: c.i.s., $\delta_{complex}$ - δ_{ligand}), ppm 7.331 (d, 2H, H_a, 7.8, -1.156), 7.185 (t, 2H, H_b, 6.8, -0.024), 7.681 (t, 2H, H_c, 7.6, -0.006), 8.948 (d, 2H, H_d, 7.8, 1.647), 2.458 (t, 2H, H_e, 10.9, -0.909), 3.773 (d, 2H, $H_{e'}$, 13.2, 0.406), 3.411 (t, 2H, H_f, 10.1, 0.437), 3.489 (d, 2H, $H_{f'}$, 8.3, 0.515), 2.339 (d, 2H, H_g, 9.8, -0.583), 3.314 (d, 2H, $H_{g'}$, 9.8, 0.392), 10.524 (d, 2H, H_2, 7.8, 1.647), 8.393 (t, 2H, H_3, 5.4, 0.529), 8.752 (d, 2H, H_4, 5.9, -0.496), 8.272 (s, 2H, H_5, 0.224).

[Ru(pdto)(dpq)](ClO_4)$_2$ 2 : δ (multiplicity, integration, assignment, J/Hz, coordination-induced shifts: c.i.s., $\delta_{complex}$ - δ_{ligand}), ppm 6.436 (d, 2H, H_a, 7.6, -2.051), 6.300 (t, 2H, H_b,

6.8, -0.909), 6.701 (t, 2H, H_c, 7.6, -0.986), 7.892 (d, 2H, H_d, 7.8, 0.591), 1.552 (t, 2H, H_e, 10.6, -1.815), 3.212 (t, 2H, $H_{e'}$, 10.8, -0.155), 2.553 (d, 2H, H_f, 6.5, -0.421), 2.875 (d, 2H, $H_{f'}$, 6.8, -0.099), 1.414 (d, 2H, H_g, 9.6, -1.508), 2.351 (d, 2H, $H_{g'}$, 9.6, -0.571), 9.730 (d, 2H, H_2, 6.2, 0.509), 7.611 (t, 2H, H_3, 6.4, -0.312), 8.885 (d, 2H, H_4, 4.4, -0.547), 8.499 (s, 2H, H_7, -0.635).

[Ru(pdto)(dppz)](ClO_4)$_2$ 3 : δ (multiplicity, integration, assignment, J/Hz, coordination-induced shifts: c.i.s., $\delta_{complex}$ - δ_{ligand}), ppm 7.353 (d, 2H, H_a, 7.3, -1.134), 7.250 (t, 2H, H_b, 6.4, 0.041), 7.692 (t, 2H, H_c, 7.7, 0.005), 9.136 (d, 2H, H_d, 7.9, 1.835), 2.475 (t, 2H, H_e, 10.5, -0.892), 4.190 (t, 2H, $H_{e'}$, 13.9, 0.823), 3.446 (d, 2H, H_f, 6.4, 0.437), 3.743 (dd, 2H, $H_{f'}$, 9.6, 9.3, 0.769), 2.294 (d, 2H, H_g, 9.6, -0.628), 3.254 (d, 2H, $H_{g'}$, 9.3, 0.332), 10.489 (d, 2H, H_2, 5.0, 1.307), 8.341 (t, 2H, H_3, 5.4, 0.436), 9.058 (d, 2H, H_4, 4.1, -0.399), 8.776 (d, 2H, H_8, 5.8, 0.447), 8.085 (t, 2H, H_9, 6.3, 0.055).

[Ru(bbdo)(phen)](ClO_4)$_2$ 4 : δ (multiplicity, integration, assignment, J/Hz, coordination-induced shifts: c.i.s., $\delta_{complex}$ - δ_{ligand}), ppm 7.307 (d, 2H, H_a, 7.8, -0.165), 6.879 (t, 2H, H_b, 7.9, -0.236), 7.053 (t, 2H, H_c, 7.6, -0.062), 7.439 (d, 2H, H_d, 8.3, -0.033), 2.694 (t, 2H, H_e, 12.2, -0.392), 3.727 (d, 2H, $H_{e'}$, 9.3, 0.641), 3.421 (t, 2H, H_f, 10.3, 0.419), 3.673 (t, 2H, $H_{f'}$, 9.0, 0.671), 2.553 (d, 2H, H_g, 9.8, -0.196), 3.284 (d, 2H, $H_{g'}$, 9.8, 0.535), 10.783 (d, 2H, H_2, 4.4, 2.213), 8.227 (t, 2H, H_3, 6.6, 0.363), 8.782 (d, 2H, H_4, 7.8, -0.466), 8.089 (s, 2H, H_5, 0.041).

[Ru(bbdo)(dpq)](ClO_4)$_2$ 5 : δ (multiplicity, integration, assignment, J/Hz, coordination-induced shifts: c.i.s., $\delta_{complex}$ - δ_{ligand}), ppm 7.105 (d, 2H, H_a, 7.4, -0.367), 6.632 (t, 2H, H_b, 6.6, -0.483), 6.789 (t, 2H, H_c, 7.6, -0.326), 7.211 (d, 2H, H_d, 8.2, -0.261), 1.842 (t, 2H, H_e, 11.6, -1.244), 3.526 (t, 2H, $H_{e'}$, 12.4, 0.440), 3.053 (d, 2H, H_f, 8.2, 0.050), 3.342 (t, 2H, $H_{f'}$, 10.6, 0.339), 1.632 (d, 2H, H_g, 9.4, -1.117), 2.553 (d, 2H, $H_{g'}$, 9.4, -0.196), 10.579 (d, 2H, H_2, 7.9, 1.358), 8.158 (t, 2H, H_3, 6.6, -0.235), 9.368 (d, 2H, H_4, 4.2, -0.044), 8.947 (s, 2H, H_7, -0.187).

[Ru(bbdo)(dppz)](ClO_4)$_2$ 6 : δ (multiplicity, integration, assignment, J/Hz, coordination-induced shifts: c.i.s., $\delta_{complex}$ - δ_{ligand}), ppm 7.074 (d, 2H, H_a, 7.8, -0.398), 7.048 (t, 2H, H_b,

6.3, -0.067), 7.190 (t, 2H, H_c, 7.5, 0.075), 8.407 (d, 2H, H_d, 8.3, 0.935), 1.590 (t, 2H, H_e, 12.9, -1.496), 3.199 (t, 2H, $H_{e'}$, 14.4, 0.113), 2.780 (d, 2H, H_f, 14.7, -0.223), 2.906 (dd, 2H, $H_{f'}$, 9.5, -0.097), 1.344 (d, 2H, H_g, 9.3, -1.405), 2.388 (d, 2H, $H_{g'}$, 9.4, -0.361), 9.399 (d, 2H, H_2, 8.0, 0.217), 8.284 (t, 2H, H_3, 6.3, 0.379), 9.131 (d, 2H, H_4, 3.5, -0.326), 8.006 (d, 2H, H_8, 6.3, -0.323), 7.870 (t, 2H, H_9, 7.1, -0.160).

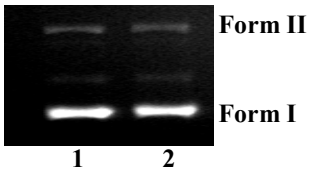

Fig. S1. Gel electrophoresis diagram showing the supercoiled pBR322 DNA (40 μM in base pair) with and without 10% DMF/5 mM Tris-HCl/50 mM NaCl buffer at pH 7.1 and 37 °C with an incubation time of 1 h. lane 1, DNA +5 mM Tris-HCl/50 mM NaCl buffer at pH 7.1; lane 2, DNA + 10% DMF/5 mM Tris-HCl/50 mM NaCl buffer. Forms I and II are supercoiled and nicked circular forms of DNA respectively.