Supplementary Material

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Non-covalent DNA binding and cytotoxicity of certain mixed ligand ruthenium(II) complexes of 2,2’-dipyridylamine and diimines

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

$^1$H NMR (DMSO-d$_6$, 400 MHz): δ (multiplicity, integration, assignment), ppm, **Hdpa**, 7.737 (d, 2H, H$_3$), 7.636 (t, 2H, H$_4$), 6.847 (t, 2H, H$_5$), 8.213 (d, 2H, H$_6$), 9.632 (s, 1H, NH); **phen**, 9.248 (dd, 2H, H$_2$), 7.864 (q, 2H, H$_3$), 8.570 (dd, 2H, H$_4$), 8.048 (s, 2H, H$_5$); **5,6-dmp**, 9.091 (d, 2H, H$_2$), 7.557 (dd, 2H, H$_3$), 8.305 (d, 2H, H$_4$), 2.574 (s, 6H, CH$_3$); **dpq**, 9.432 (d, 2H, H$_2$), 7.923 (dd, 2H, H$_3$), 9.221 (d, 2H, H$_4$), 9.134 (s, 2H, H$_6$); **mdpq**, 9.466 (dd, 2H, H$_2$), 7.862 (dd, 2H, H$_3$), 9.211 (dd, 2H, H$_4$), 9.036 (s, 1H, H$_6$), 2.798 (s, 3H, CH$_3$); **dppz**, 9.457 (d, 2H, H$_2$), 7.905 (t, 2H, H$_3$), 9.182 (d, 2H, H$_4$), 8.329 (d, 2H, H$_7$), 8.030 (t, 2H, H$_8$).
Fig. S1 $^1$H NMR spectrum of [Ru(Hdpa)$_2$(phen)]$^{2+}$ 1 in (CD$_3$)$_2$SO.

Fig. S2 The chemical shift patterns of [Ru(Hdpa)$_2$(phen)]$^{2+}$ 1 compared with their corresponding tris analogues and 2-5. (A) ● : [Ru(phen)$_3$]$^{2+}$; ▲ : [Ru(Hdpa)$_3$]$^{2+}$; ○ : Group I; □ : Group II; ♦ : Group III. (B) Comparison of the chemical shift patterns of H$_2$, H$_3$ and H$_4$ protons of Group I. ● : phen (1); × : 5,6-dmp (2); ○ : dpq (3); ▲ : mdpq (4); □ : dppz (5). (C) Comparison of the chemical shift patterns of Group II. ▲ : 1; □ : 2; ○ : 3; × : 4; ♦ : 5. (D) Comparison of the chemical shift patterns of Group III. ▲ : 1; □ : 2; ○ : 3; × : 4; ♦ : 5.