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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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^{1}H NMR (DMSO-d_6, 400 MHz)

The chemical shifts of the free and coordinated ligands are summarized 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 ^{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).

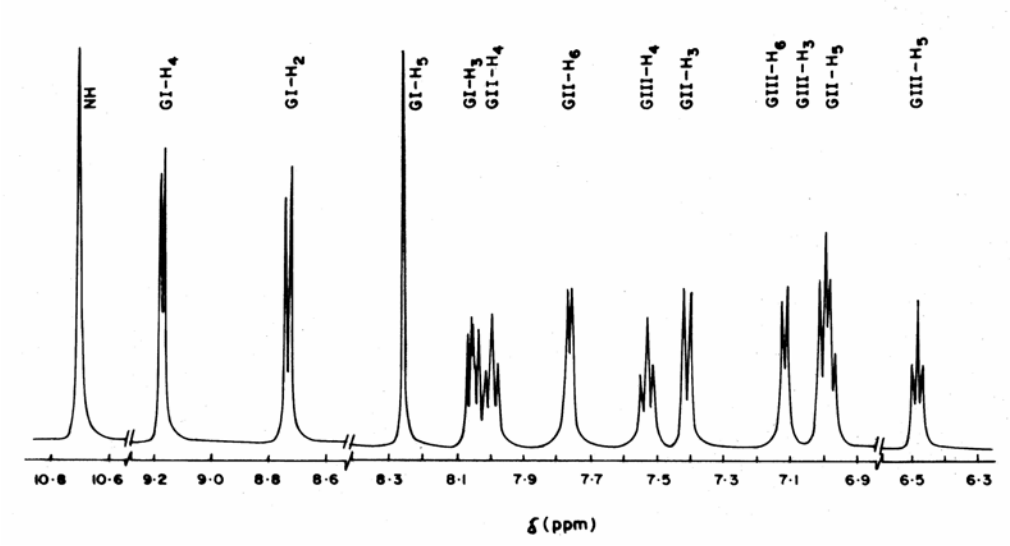

Fig. S1 ^{1}H NMR spectrum of $[Ru(Hdpa)_2(phen)]^{2+}$ **1** in $(CD_3)_2SO$.

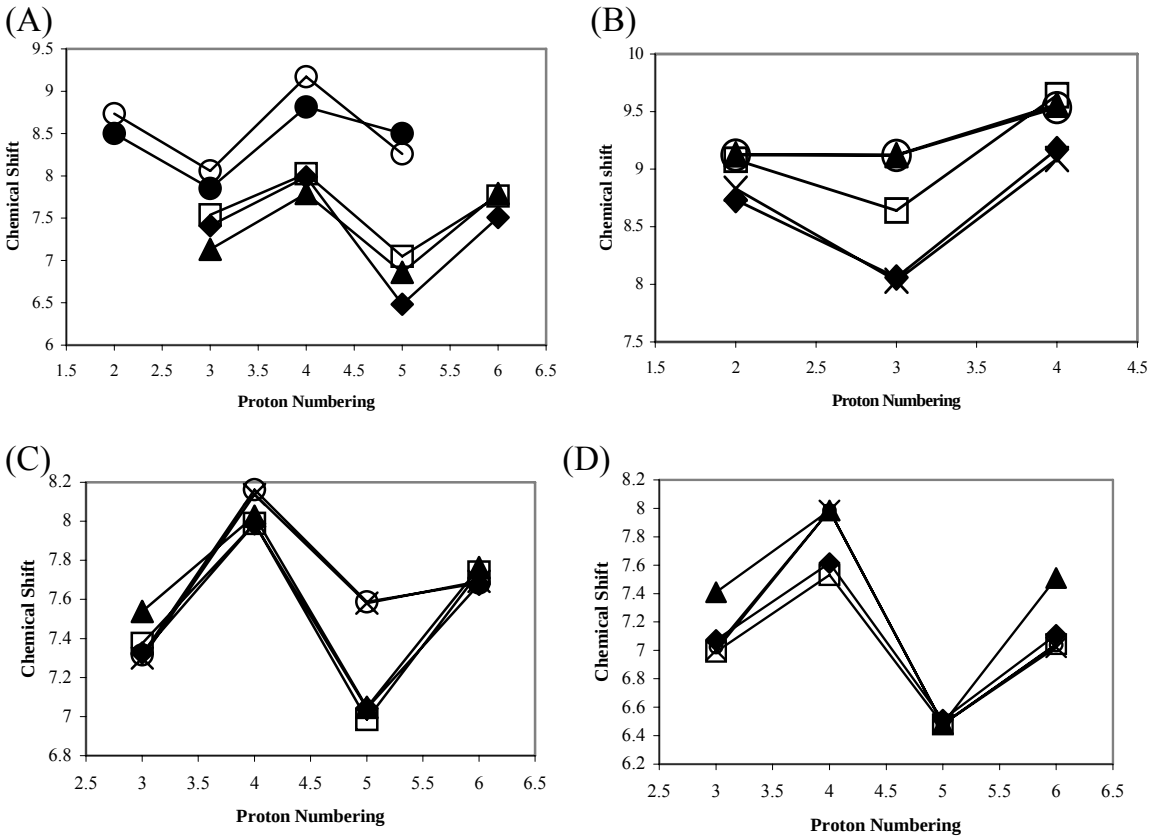

Fig. S2 The chemical shift patterns of $[Ru(Hdpa)_2(phen)]^{2+}$ **1** compared with their corresponding tris analogues and **2**-**5**. (A) ●: $[Ru(phen)_3]^{2+}$; ▲ : $[Ru(Hdpa)_3]^{2+}$; ○ : Group I; □ : Group II; ♦ : Group III. (B) Comparison of the chemical shift patterns of H_2, H_3 and H_4 protons 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**.