Supplementary Information

Structural, electrochemical, phosphate-hydrolysis, DNA binding and cleavage studies of new macrocyclic binuclear nickel(II) complexes

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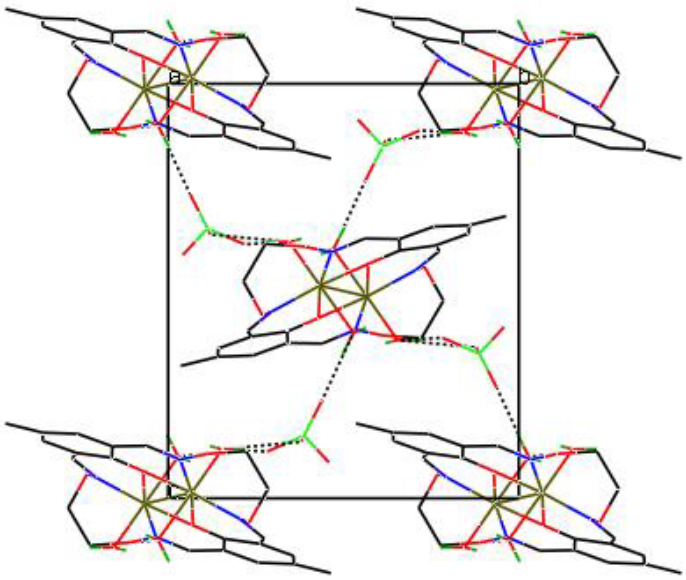

Fig. S1 The crystal packing of the macrocyclic binuclear Ni(II) complex **1**, viewed down the 'a' axis. C-bound H atoms have been omitted for the sake of clarity

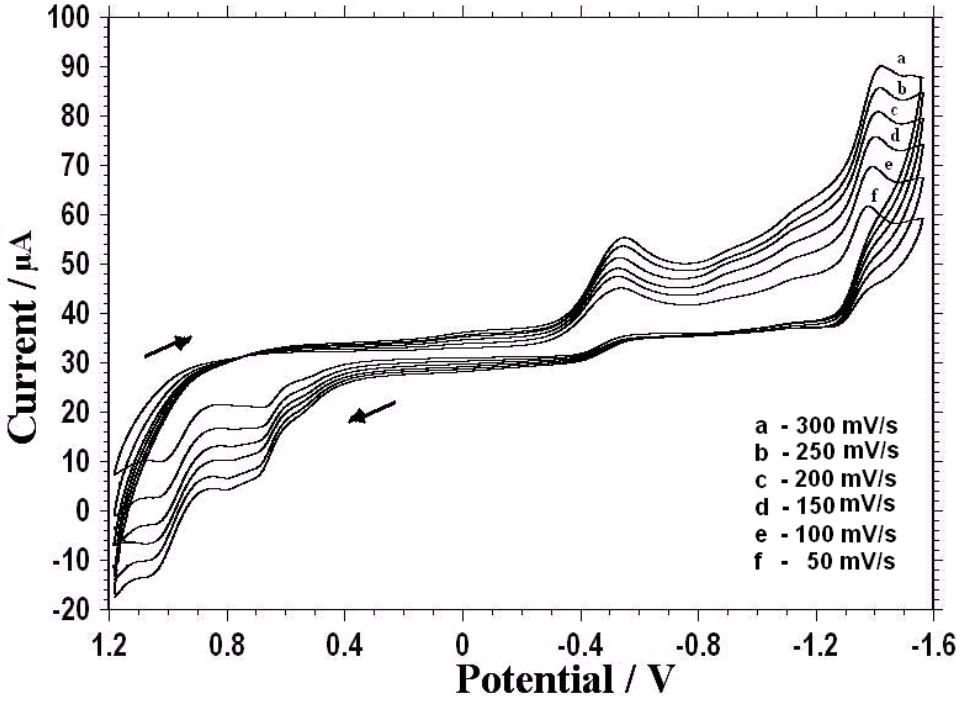

Fig. S2 Cyclicvoltammogram of **1** in CH_3CN

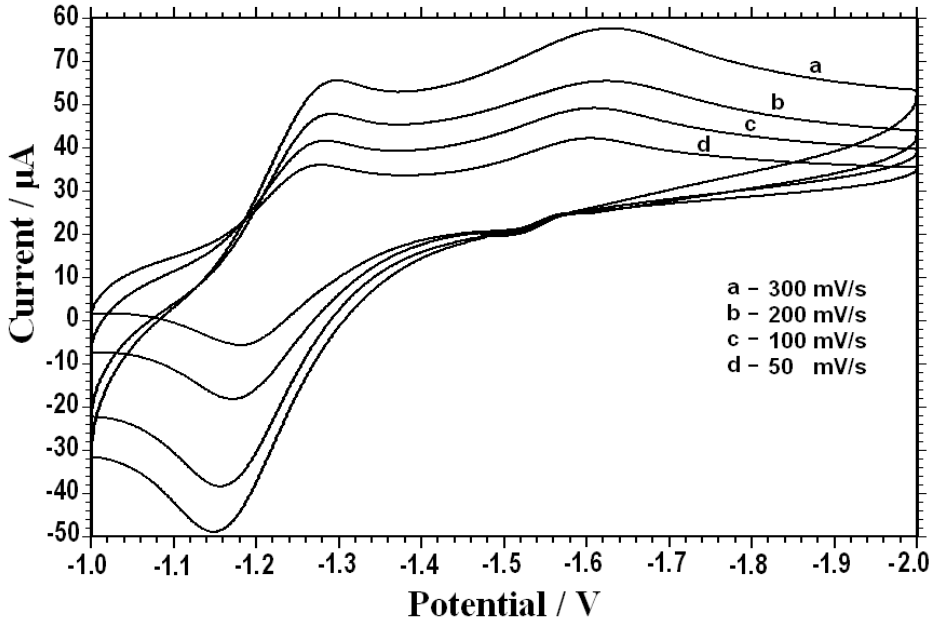

Fig. S3 Cyclicvoltammogram of **5** (cathodic region) in CH_3CN

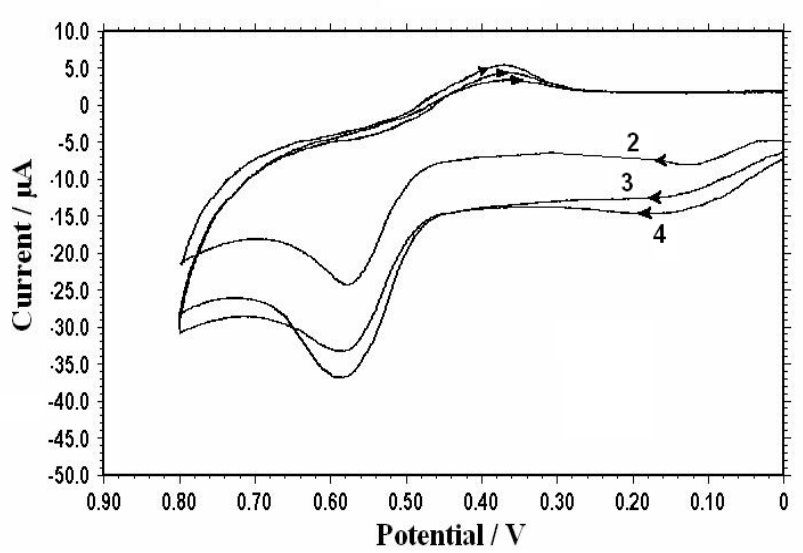

Fig. S4 Cyclicvoltammogram of **2-4** (Anodic region) in CH_3CN

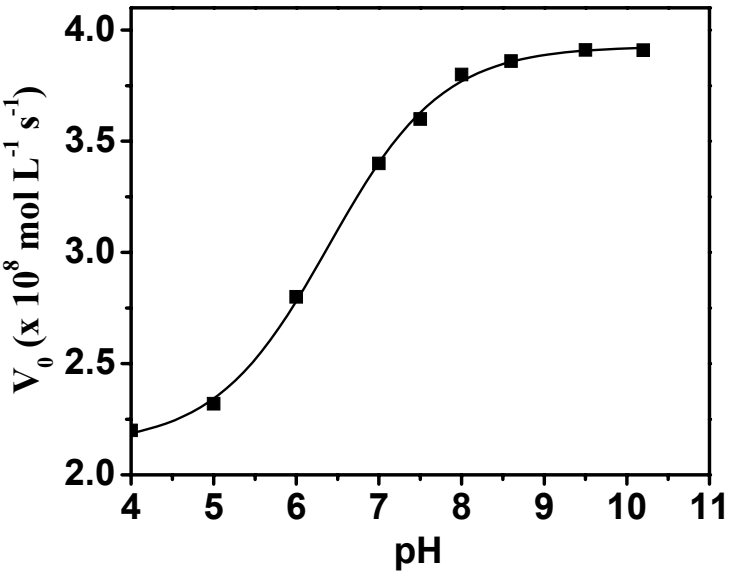

Fig. S5 Dependence of the reaction rates on pH Hydrolysis of 4-NPP by macrocyclic binuclear Ni(II) complex **1**

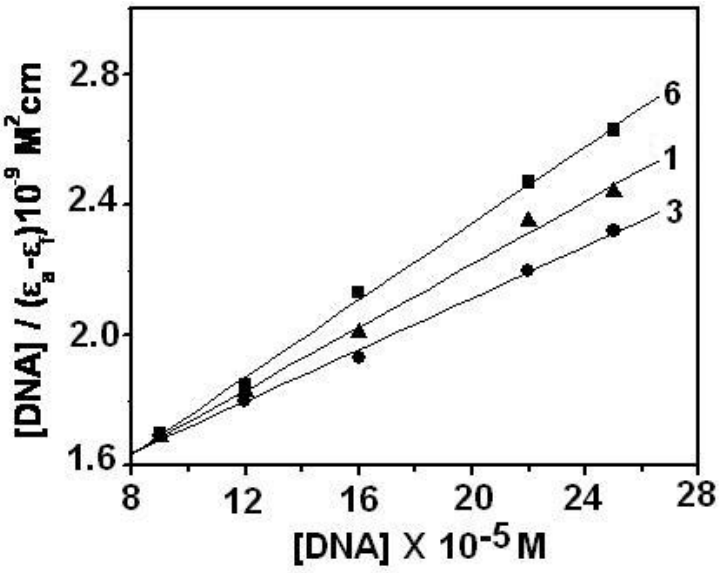

Fig. S6 The plots of [DNA] / (ϵ_a-ϵ_f) versus [DNA] for the titration of DNA with Ni(II) complexes **1, 3** and **6**.

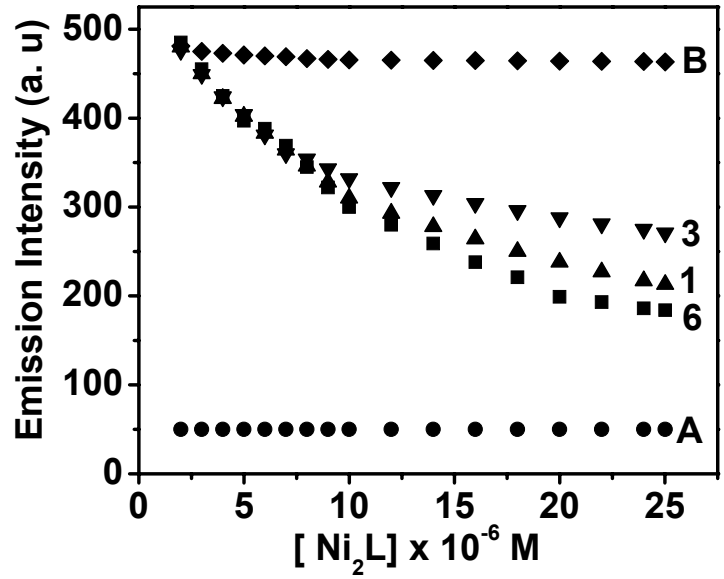

Fig. S7 The effect of addition of complexes **1**, **3** and **6** on the emission intensity of 40 μM CT DNA-bound EB in Tris-HCl/NaCl buffer (50 mM, pH 7.5) at 25 ˚C; (**A**) on the emission intensity of the EB in absence of CT DNA but at different concentrations of complexes (**1**, **3** & **6)** and nickel(II) perchlorate hexahydrate (**B**).

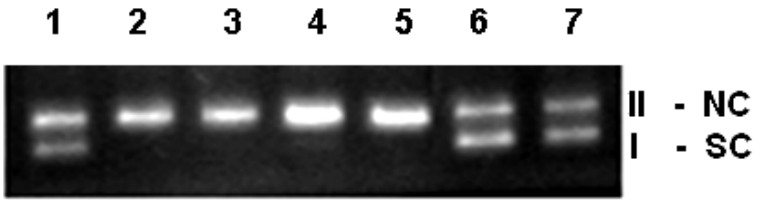

Fig. S8 Cleavage mechanism of SC pBR322 DNA (33 μM) by Ni(II) complexes **1** and **6** (50 μM) in the presence of H_2O_2 (40 μM) in 50 mM Tris-HCl / NaCl buffer (pH 7.2). Lanes 1, DNA control; 2, DNA + H_2O_2 + 3 + DMSO (70 mM); 3, DNA + 6 + DMSO (70 mM), 4, DNA + H_2O_2 + 3 + SOD (4 units); 5, DNA + H_2O_2 + 6 + SOD (4 units); 6, DNA + H_2O_2 + 3 + EDTA (50 mM); 6, DNA + H_2O_2 + 6 + EDTA (50 mM).

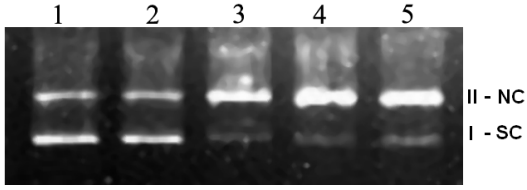

Fig. S9 Anaerobic cleavage of SC pBR322 DNA (33 μM) by complex **1**, **5** and **6** incubated for 3 h under argon atmosphere (pH 7.2) at 21˚C . Lanes 1, DNA control; 2, DNA + H_2O_2; 3, DNA + H_2O_2 + 1 ; 4, DNA + H_2O_2 + 5; 5, DNA + H_2O_2 + 6.

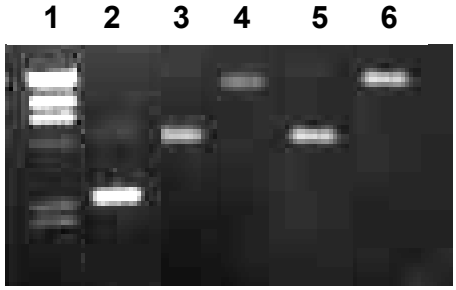

Fig. S10 Gel electrophoresis diagram for ligation of SC pBR322 DNA nicked by 5 and 6. Lanes 1, λHindIII markers; 2, DNA control; 3 and 4, linear form (from DNA + 5) as control without and with T4 ligase (4 units); 3 and 4, linear form (from DNA + 6) without and with T4 ligase.