

Supporting Information for:

**Binding of $[\text{Pt}(\text{1C3})(\text{dien})]^{2+}$ to the duplex DNA oligonucleotide
5'-d(TGGCCA)-3': the effect of an appended positive charge on the
orientation and location of anthraquinone intercalation**

Renee M. Whan, Barbara A. Messerle, and Trevor W. Hambley*

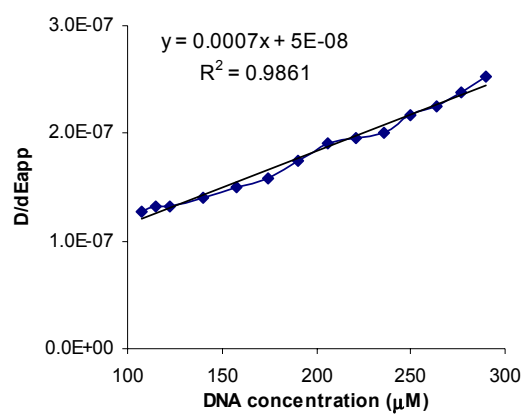
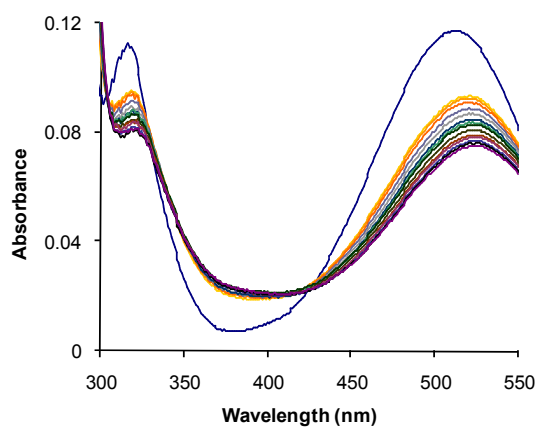
School of Chemistry, The University of Sydney, NSW 2006, Australia

*Corresponding author:

t.hambley@chem.usyd.edu.au

ph: 61-2-9351-2830

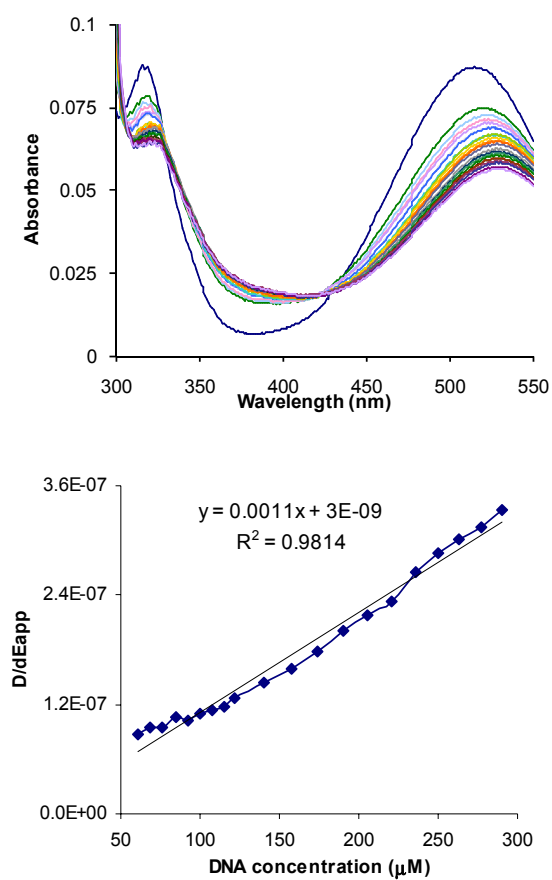
fax: 61-2-9351-3329



A

B

Figure S1: **A** shows the UV-spectrophotometric titration curves and **B** shows the half reciprocal plot obtained from titrating 1C3 (20 μM) with salmon sperm DNA.



A

B

Figure S2: **A** shows the UV-spectrophotometric titration curves and **B** shows the half reciprocal plot obtained from titrating $[\text{Pt}(\text{1C3})(\text{dien})]^{2+}$ (20 μM) with salmon sperm DNA.

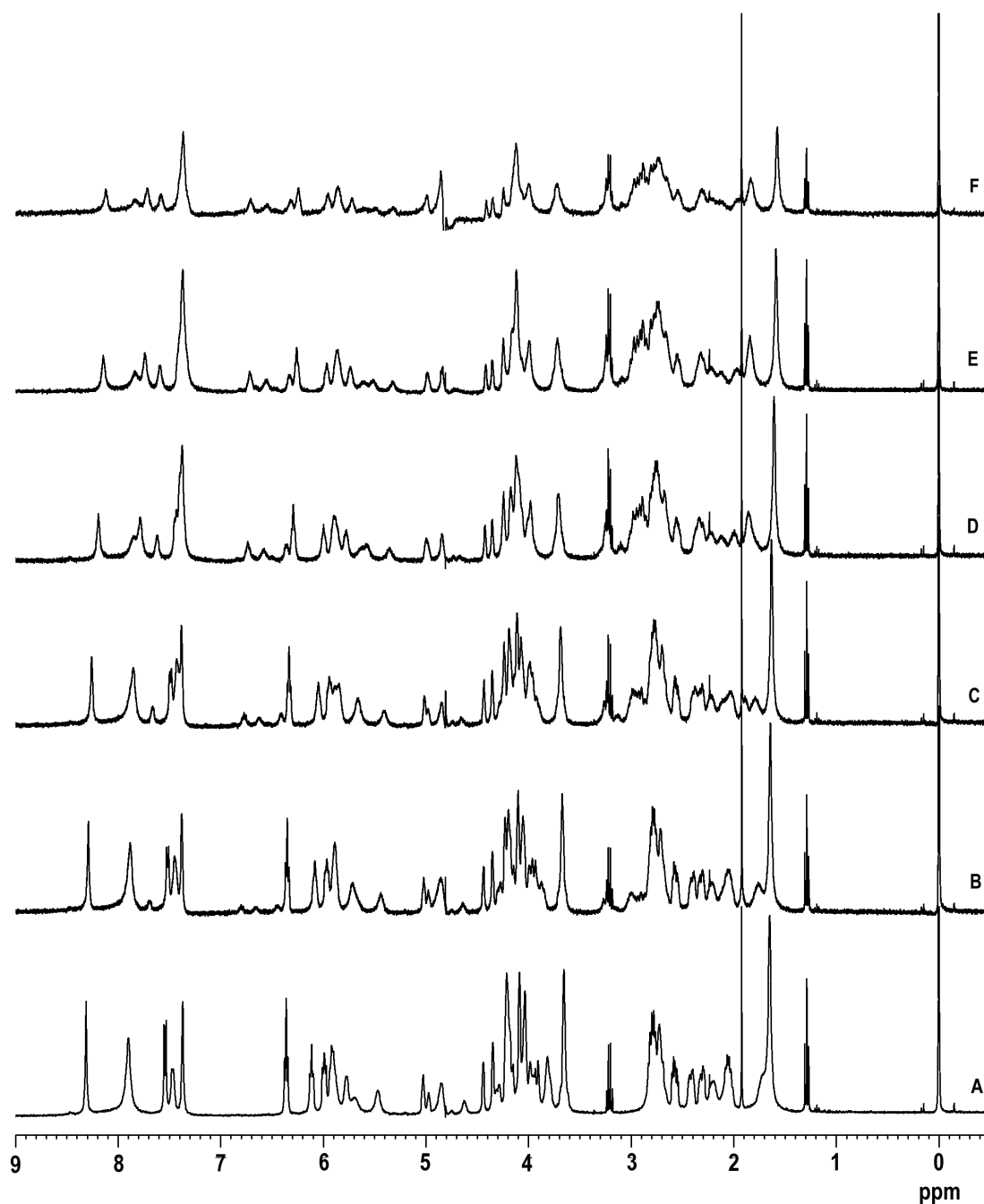


Figure S3: The 1D ^1H NMR spectra (400 MHz) of a sample of TGGCCA titrated with $[\text{Pt}(\text{1C3})(\text{dien})]^{2+}$ at 298K to form the 1:2 complex. A is the duplex hexamer alone, B is a TGGCCA: $[\text{Pt}(\text{1C3})(\text{dien})]^{2+}$ ratio of 2.5:1, C is 1:1, D is 1:1.4, E is 1:1.9 and F is 1:2.

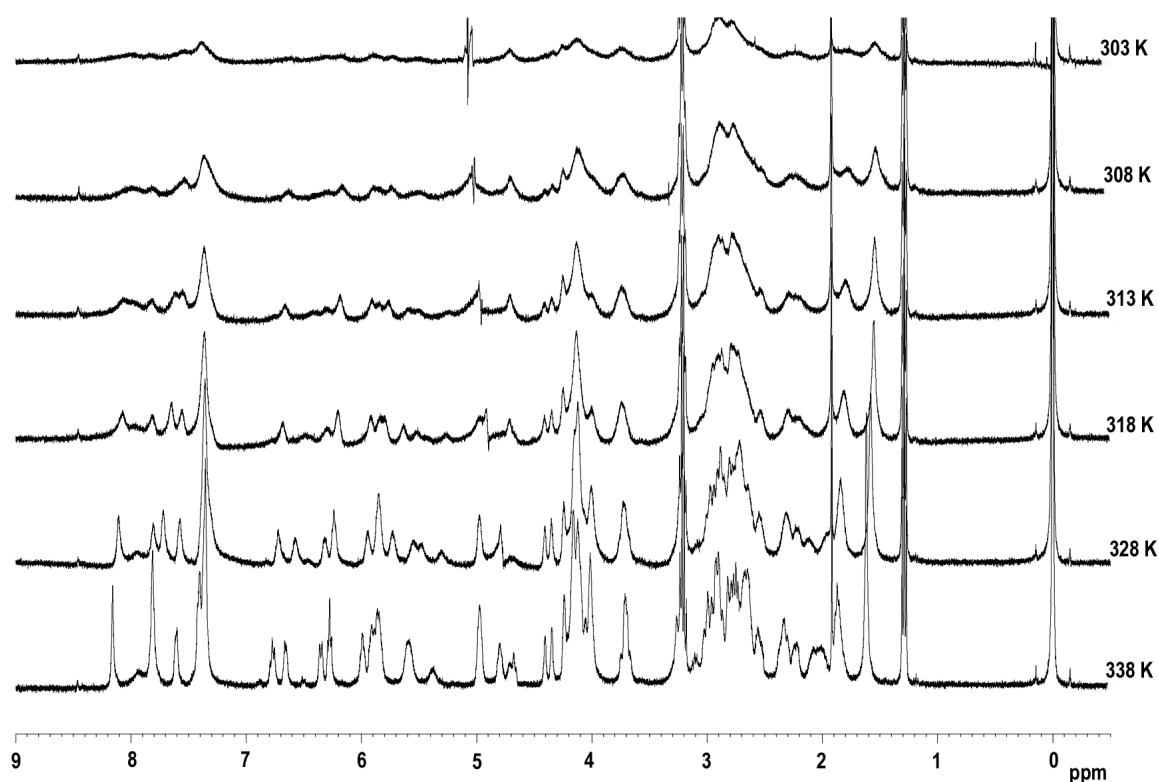


Figure S4: The effect of temperature on the 1D ¹H NMR spectra (400 MHz) of a sample of TGGCCA that had been titrated with [Pt(1C3)(dien)]²⁺, where the ratio of TGGCCA:[Pt(1C3)(dien)]²⁺ is 1:2.

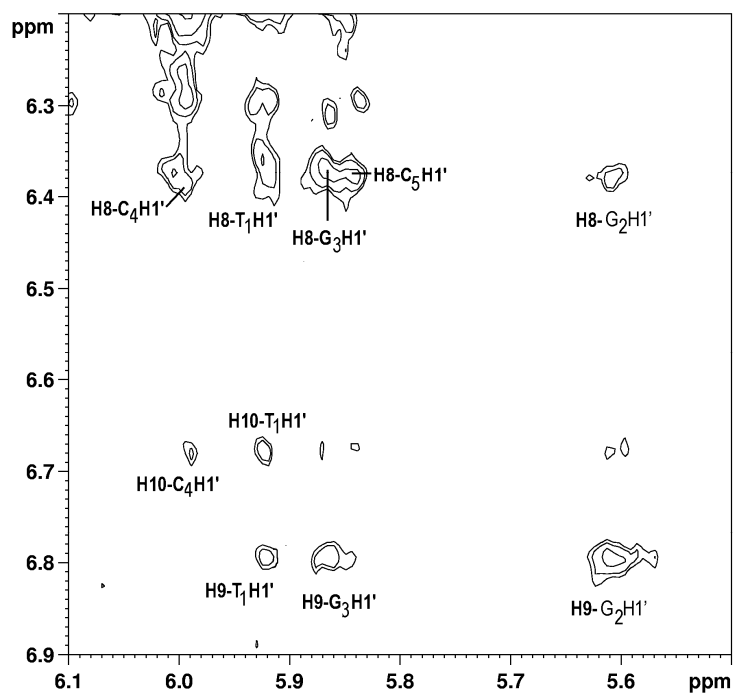


Figure S5: 2D NOESY spectrum of a mixture of TGGCCA and $[\text{Pt}(\text{1C3})(\text{dien})]^{2+}$ in a 1:2 ratio. The spectrum shows the crosspeaks occurring due to interaction between the aromatic protons of the anthraquinone and the H1' sugar protons.

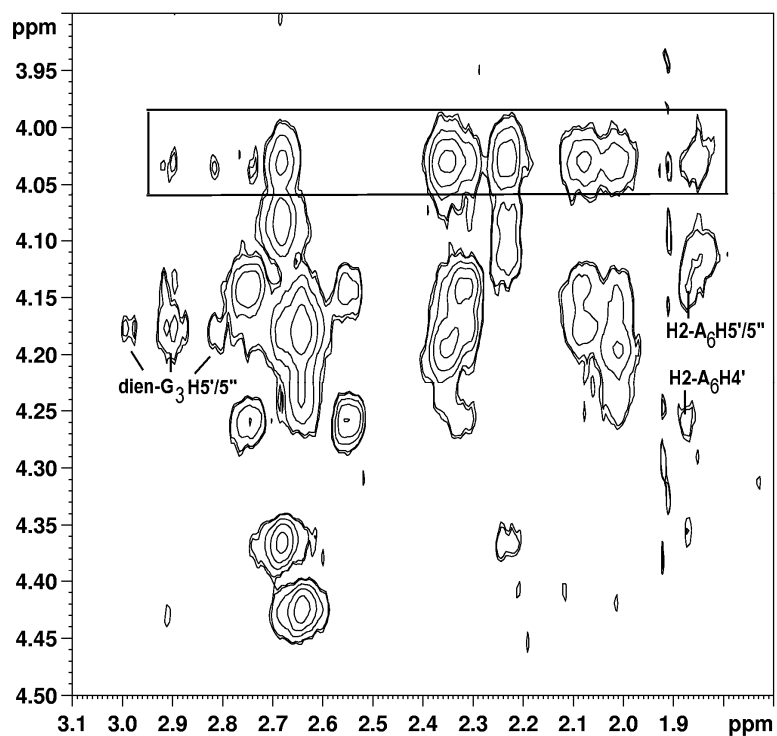


Figure S6: 2D NOESY spectrum of a mixture of TGGCCA with $[\text{Pt}(\text{1C3})(\text{dien})]^{2+}$ in a 1:2 ratio. The spectrum shows the crosspeaks occurring due to interactions between the protons of the platinum complex and the H4', H5' and H5'' sugar protons. The boxed area shows the direct overlap of the G2 and C5 H5' and H5'' resonances.