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Cadmium(II) complexes of 5-nitro-salicylaldehyde and α-diimines: Synthesis, structure and interaction with calf-thymus DNA

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S1. Interaction with CT DNA

The binding constant, K_b, can be obtained by monitoring the changes in the absorbance at the corresponding λ_{max} with increasing concentrations of CT DNA and it is given by the ratio of slope to the y intercept in plots $\frac{[DNA]}{(\varepsilon_A - \varepsilon_f)}$ versus [DNA], according to the Wolfe–Shimer equation [S1]:

$$\frac{[DNA]}{(\varepsilon_A - \varepsilon_f)} = \frac{[DNA]}{(\varepsilon_b - \varepsilon_f)} + \frac{1}{K_b(\varepsilon_b - \varepsilon_f)} \qquad \text{(eq. S1)}$$

where [DNA] is the concentration of DNA in base pairs, $\varepsilon_A = A_{obsd}$/[compound], ε_f = the extinction coefficient for the free compound and ε_b = the extinction coefficient for the compound in the fully bound form.

S2. Competitive studies with EB

The Stern–Volmer constant K_{SV} is used to evaluate the quenching efficiency for each compound according to the Stern–Volmer equation [S2]:

$$\frac{Io}{I} = 1 + K_{SV}[Q] \qquad \text{(eq. S2)}$$

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where Io and I are the emission intensities in the absence and the presence of the quencher, respectively, [Q] is the concentration of the quencher (i.e. complexes **1–5**); K_{SV} is obtained from the Stern–Volmer plots by the slope of the diagram $\frac{Io}{I}$ vs [Q].

References

[S1] A. Wolfe, G. Shimer, T. Meehan, *Biochemistry*, **26**, 6392 (1987).

[S2] J.R. Lakowicz, *Principles of Fluorescence Spectroscopy*, 3rd Edn., Plenum Press, New York (2006).

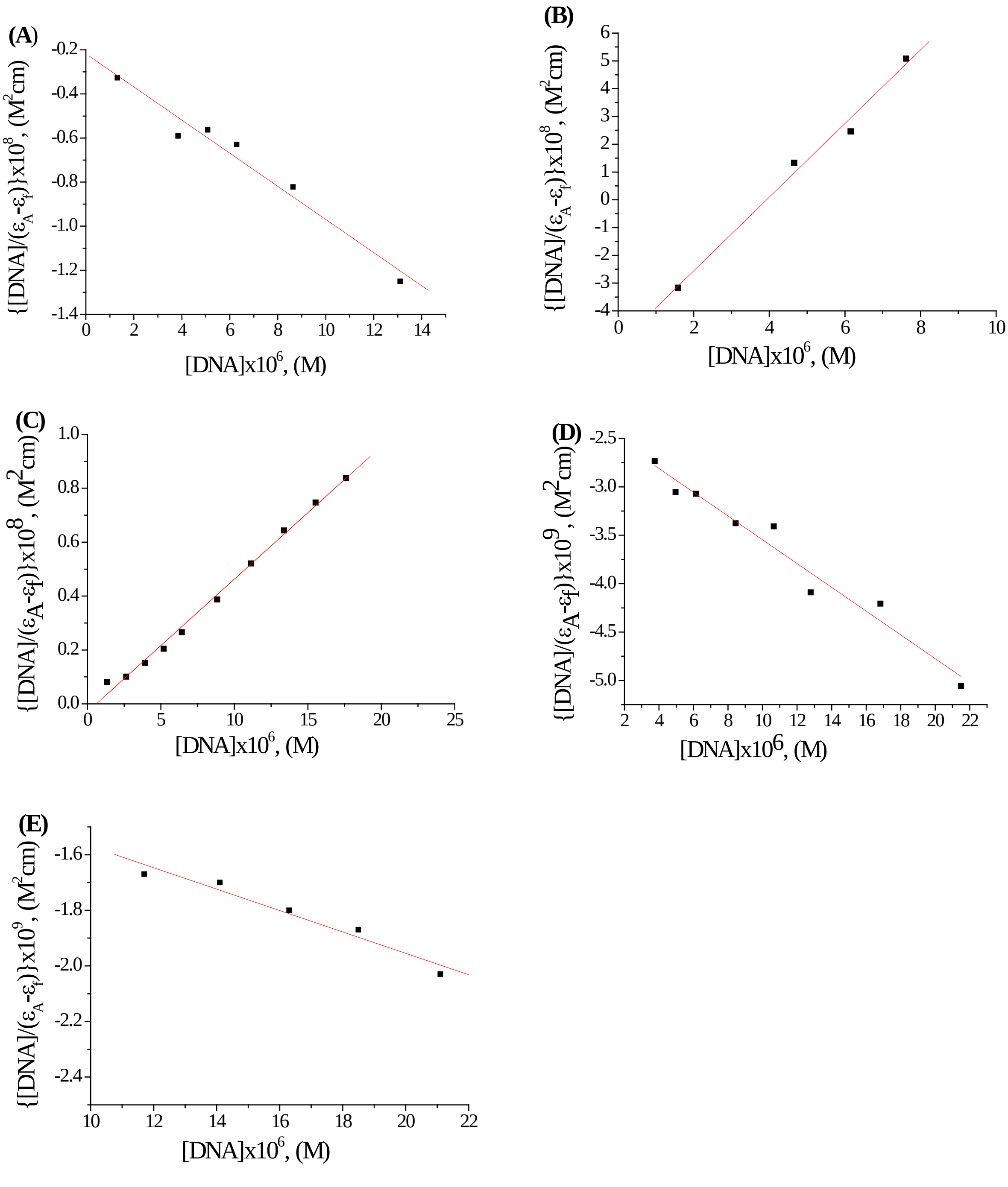

Fig. S1. (A)–(E) Plot of $\frac{[DNA]}{(\varepsilon_A - \varepsilon_f)}$ vs [DNA] for complexes **1–5**, respectively.

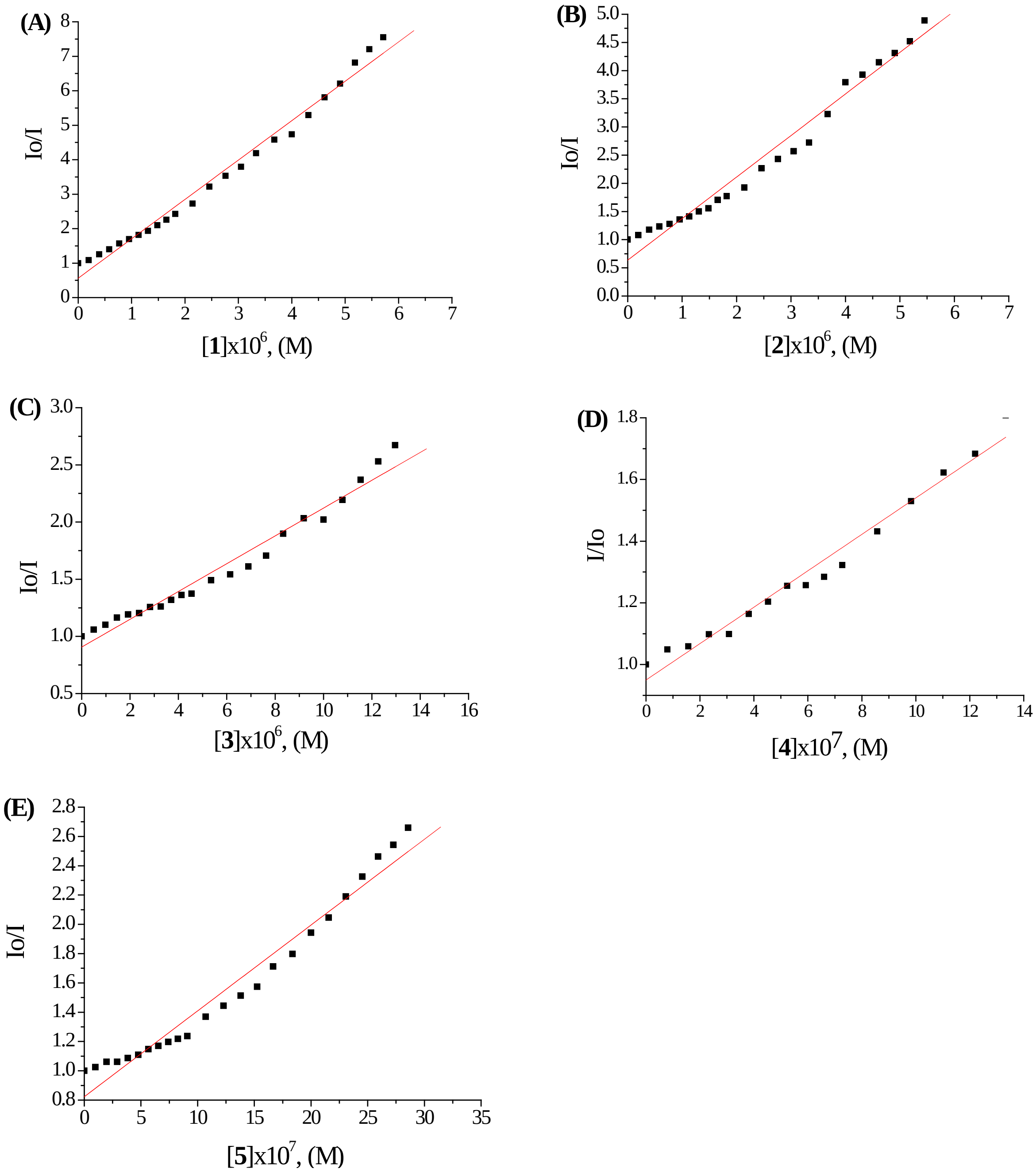

Fig. S2. (A)–(E) Stern–Volmer quenching plot of EB bound to CT DNA for complexes **1–5**, respectively.