Binding of an anionic fluorescent probe with calf thymus DNA and effect of salt on the probe-DNA binding: A spectroscopic and molecular docking investigation

Saptarshi Ghosh^a, Pronab Kundu^a, Bijan Kumar Paul^b, and Nitin Chattopadhyay^{a,*}

^aDepartment of Chemistry, Jadavpur University, Kolkata - 700 032, India ^bDepartment of Chemistry, Indian Institute of Science Education and Research Bhopal, Bhauri, Bhopal 462066, Madhya Pradesh, India

*Corresponding author: Fax: 91-33-2414 6584 E-mail: <u>nitin.chattopadhyay@yahoo.com</u>

Electronic Supplementary Information



Fig. S1 Double reciprocal plot for the binding of ANS and ctDNA from absorption data.



Fig. S2 Fluorescence spectra of ctDNA bound EtBr with the addition of varying concentrations of ANS. Concentrations of ANS are labeled in the legends; $\lambda_{exc} = 480$ nm. [ctDNA] = 1 mM and [EtBr] = 10 μ M. Inset shows the emission spectra of the same solutions in the lower wavelength range; $\lambda_{exc} = 370$ nm.



Fig. S3 Emission spectra of ANS in the presence of different concentrations of NaCl. The concentrations of the NaCl solutions are labeled in the legends. $\lambda_{exc} = 370$ nm. [ANS] = 10 μ M.



Fig. S4 Variation of the anisotropy of the ctDNA bound ANS as a function of concentration of NaCl. $\lambda_{exc} = 370 \text{ nm}, \lambda_{em} = 500 \text{ nm}. \text{ [ctDNA]} = 1.92 \text{ mM} \text{ and [ANS]} = 10 \text{ }\mu\text{M}.$



Fig. S5 Emission profile of ctDNA bound ANS with increasing NaBr concentration. The concentrations of the NaBr solutions are labeled in the legends. $\lambda_{exc} = 370$ nm. [ctDNA] = 1.92 mM and [ANS] = 10 μ M.



Fig. S6 Emission profile of ctDNA bound ANS with increasing NaI concentration. The concentrations of the NaI solutions are labeled in the legends. $\lambda_{exc} = 370$ nm. [ctDNA] = 1.92 mM and [ANS] = 10 μ M.