

SUPPLEMENTARY MATERIAL TO
**Binding elucidation of azo dye with DNA via spectroscopic
approaches and molecular docking techniques**

SHABNAM JAMPOUR-KOLOUR and HAMID DEZHAMPANAH*

*Department of Applied Chemistry, Faculty of Chemistry, University of Guilan, P.O.B. 1914,
Rasht 0098, Iran*

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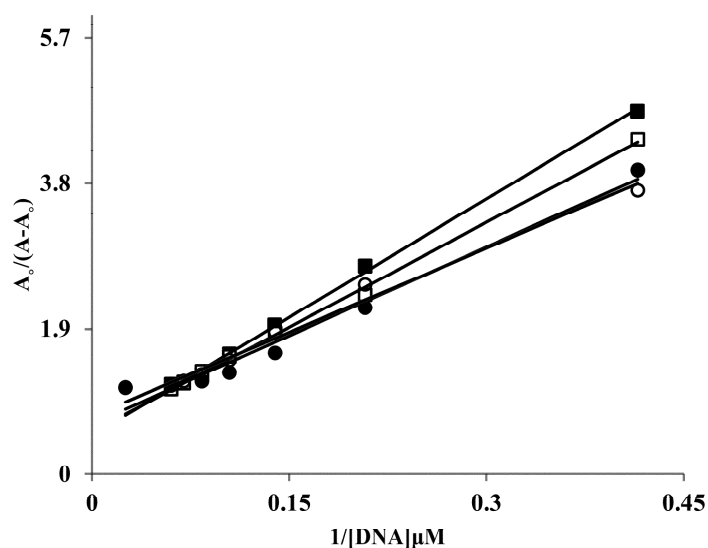


Fig. S-1. Benesi Hildbrand plots for the interactions of Ct-DNA-BAE. (■298.2K, □ 303.2K, ○ 313.2K, ● 318.2K)

* Corresponding author. E-mail: h.dpanah@guilan.ac.ir

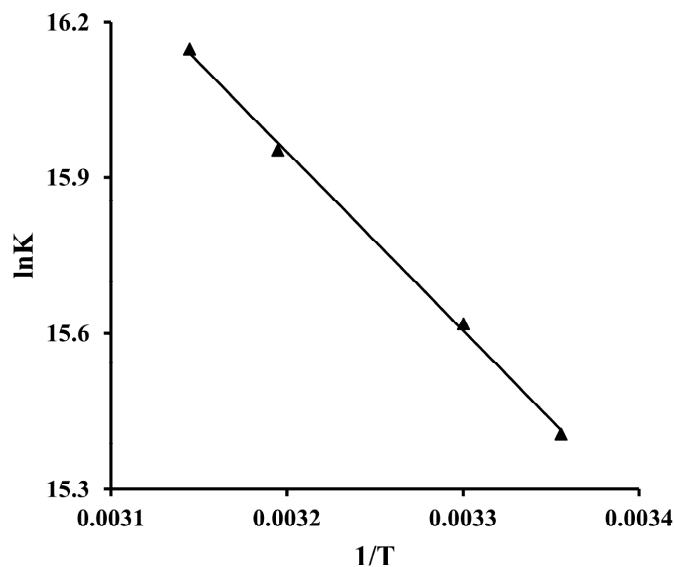


Fig. S-2. Plots of $\ln K$ vs. $1/T$ for the determination of thermodynamic parameters.

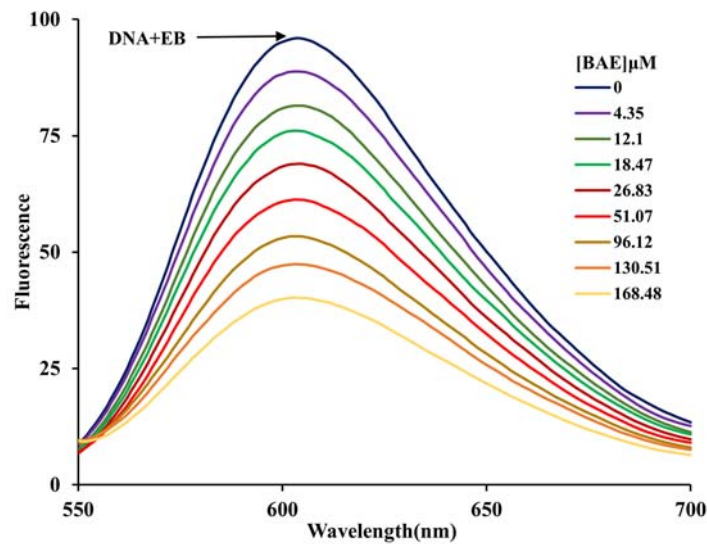


Fig. S-3. Fluorescence quenching EB-Ct-DNA system in the absence and presence of BAE: $[Ct-DNA] = 160 \mu M$, $[EB] = 320 \mu M$, and $[BAE]$ azo dye from 0 to 168 μM .

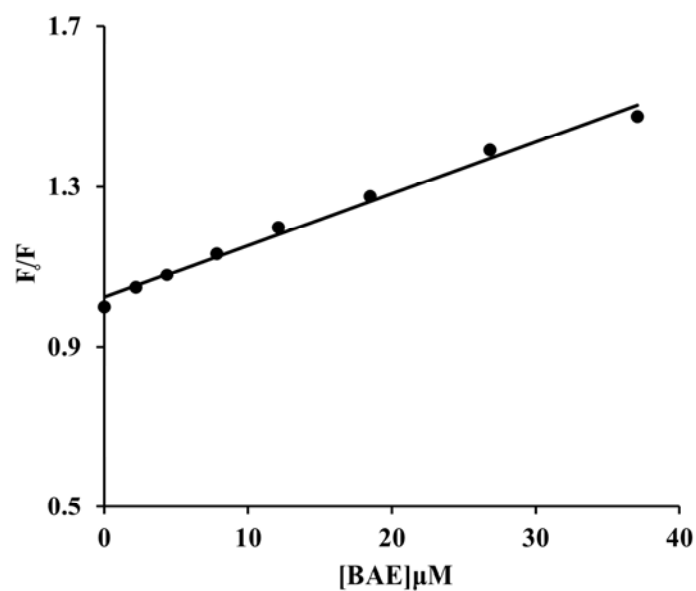


Fig. S-4. Linear Stern–Volmer plot of the EB-Ct-DNA system in the absence and presence of BAE at 298.2 K.

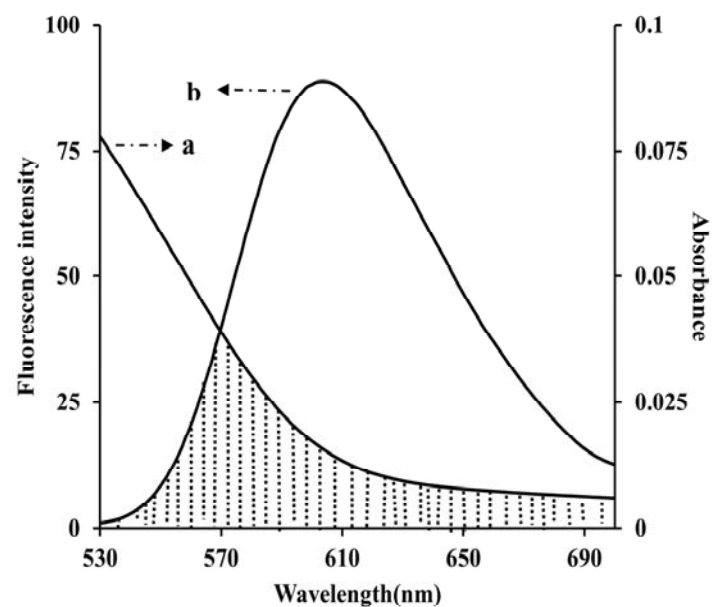


Fig. S-5. Overlap of the absorption spectra of BAE (a) with fluorescence emission of Ct-DNA-EB (b) in 5 mM phosphate buffer, pH = 7.2, at 298.2 K, $\lambda_{ex} = 450$ nm $[BAE] = [Ct-DNA-EB] = 12.10 \mu M$.

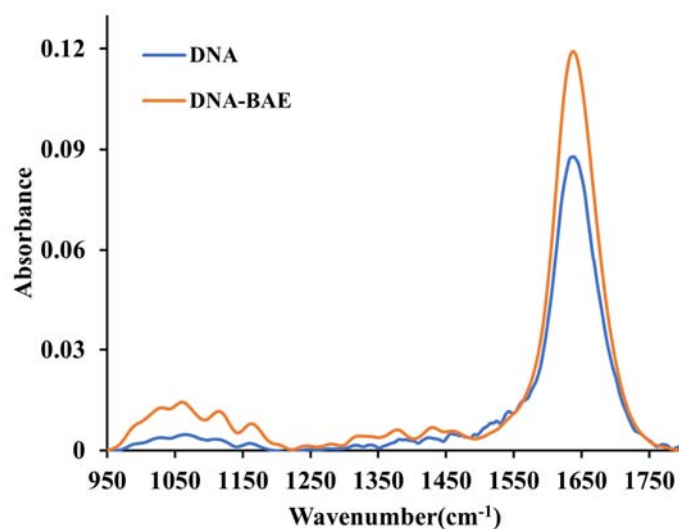


Fig. S-6. FT-IR spectra of the BAE-Ct-DNA system. The concentration of Ct-DNA was fixed at 500 μM , and the BAE concentration was fixed at 40 μM .

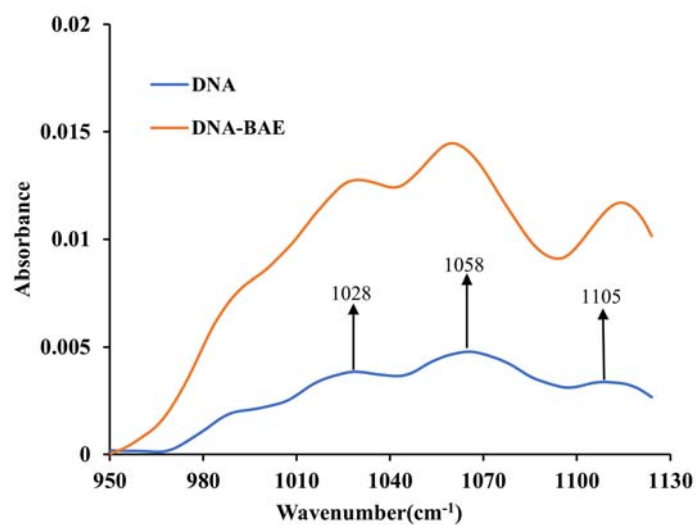


Fig. S-7. Highlights of the FT-IR spectra of the BAE-Ct-DNA system at 950-1130 cm^{-1} region. The concentration of Ct-DNA was fixed at 500 μM , and the BAE concentration was fixed at 40 μM .

TABLE S-I. the relative contribution of bands to the total absorption in 1750–1550 cm^{-1} region in %

Peak	Ct-DNA%	Ct-DNA-BAE%
1688	11.98	16.67
1673	7.02	6.54
1658	12.75	13.08
1641	29.84	26.16
1619	23.88	22.76
1579	7.52	5.03
1573	7.01	9.45

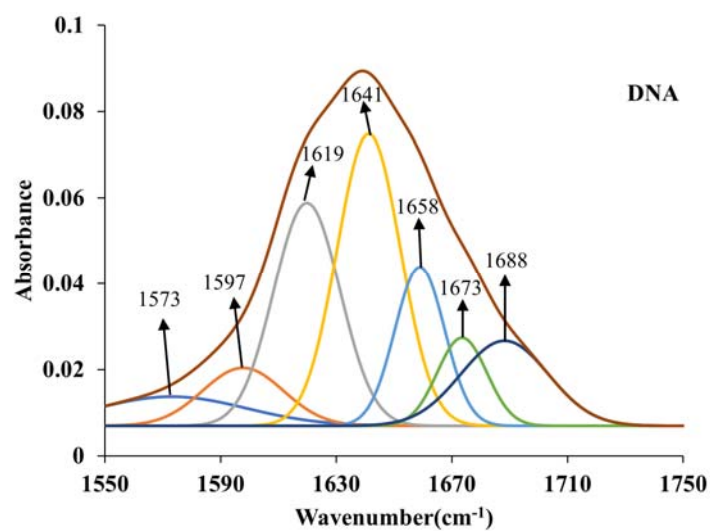


Fig. S-8. FT-IR spectra, Gaussian function fitting curves and deconvoluted spectra Ct-DNA band region (1550–1750 cm^{-1}) at 298 K and pH = 7.2.

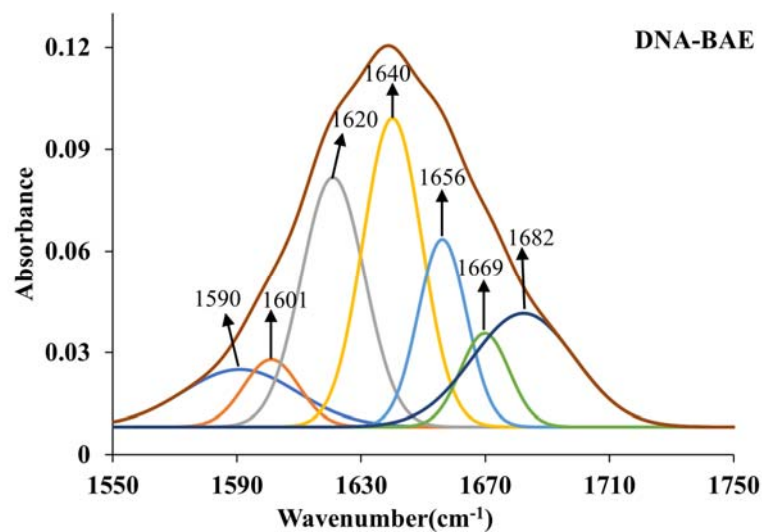
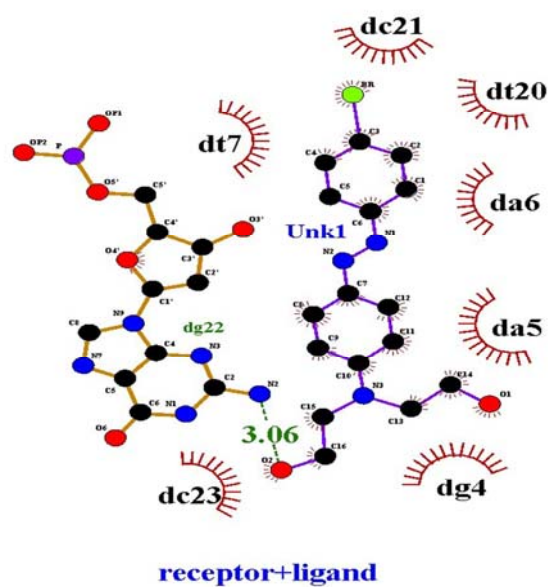


Fig. S-9. FT-IR spectra, Gaussian function fitting curves and deconvoluted spectra Ct-DNA-BAE band region (1550–1750 cm^{-1}) at 298 K and pH = 7.2.



The meaning of the items on the plot is as follows:

- | | | | |
|--|------------------------------|--|---|
| | Ligand bond | | His 53 Non-ligand residues involved in hydrophobic contact(s) |
| | Non-ligand bond | | Corresponding atoms involved in hydrophobic contact(s) |
| | Hydrogen bond and its length | | |

Fig. S-10. Hydrophobic interactions and hydrogen bonds in the interaction model of BAE with Ct-DNA