Electronic Supplementary Information

Impact of cationic surfactant-induced DNA compaction on the characteristics of the minor groove bound flavonol

Dipanjan Halder and Pradipta Purkayastha*

Department of Chemical Sciences and Center for Advanced Functional Materials, Indian Institute of Science Education and Research Kolkata, Mohanpur 741246, WB, India.

MATERIALS AND METHODS

Materials

3-HF, CTAB, ct-DNA (molecular weight 8.4 MDa) and ethanol were purchased from Sigma-Aldrich, and the HEPES buffer was obtained from SRL, India. The solutions were prepared using ultrapure water from Merck, India.

Preparation of solutions

7 mM 3-HF stock solution was prepared in spectroscopic grade ethanol. 20 μM 3-HF, prepared in HEPES buffered solution (pH 7.4), was used for all the measurements. Concentration of ethanol in the final solution was less than 1%. 10 mM CTAB stock solution was prepared in water. 3 mM stock solution of ct-DNA was prepared in HEPES buffer (pH 7.4) and stored at 4^{o}C. The concentration of ct-DNA was calculated in a spectrophotometer using ε_{DNA} = 6600 $mol^{-1}dm^{3}cm^{-1}$ at 260 nm.

Methods of measurements

The absorption spectra were recorded in a Hitachi U-2900 spectrophotometer. Steady state fluorescence and anisotropy measurements were done in a QM-40 spectrofluorimeter from PTI. The fluorescence anisotropy (r) is defined as:

$$r = \frac{(I_{VV} - GI_{VH})}{(I_{VV} + 2GI_{VH})}$$

where, I_{VV} and I_{VH} are the emission intensities of the excitation polarizer oriented vertically and emission polarizer oriented vertically and horizontally, respectively. The G factor is defined as:

$$G = \frac{I_{HV}}{I_{HH}}$$

where, I_{HV} and I_{HH} intensities refer to the vertical and horizontal positions of the emissions polarizer keeping the excitation polarizer horizontal.

The CD spectra were recorded in a JASCO J-815 spectrometer using a quartz cuvette with 1 mm path length in the wave length range 200-500 nm. The CD profiles were obtained employing a scan rate of 100 nm/min against a corrected baseline with the buffer solution.

A ZEISS (Supra) instrument was used for taking the scanning electron microscopy (SEM) images. The fluorescence microscopic images were taken from a motorized inverted research microscope (Olympus IX81) with fluorescence and DIC optics. 460-495 nm lasers were used for excitation and emission the between 510-550 nm was collected.

The time-resolved fluorescence decay data were obtained using the time correlated single photon counting (TCSPC) method. The fluorescence decay and the anisotropy data were measured from a Horiba Jobin Yvon time-resolved spectrometer with a 375 nm diode laser excitation (temporal resolution <70 ps). The raw data of fluorescence decay were fitted by a non-linear least square iteration procedure using IBH DAS6 (version 2.2) software. The time-resolve fluorescence anisotropy, r(t) could be determined by using the same equation used for steady state anisotropy. The change in anisotropy with the time is given by:

$$r(t) = r_0 e^{\left(-t/\tau_r\right)}$$

where, r_0 is the initial anisotropy and the rotational correlation time was denoted by τ_r.

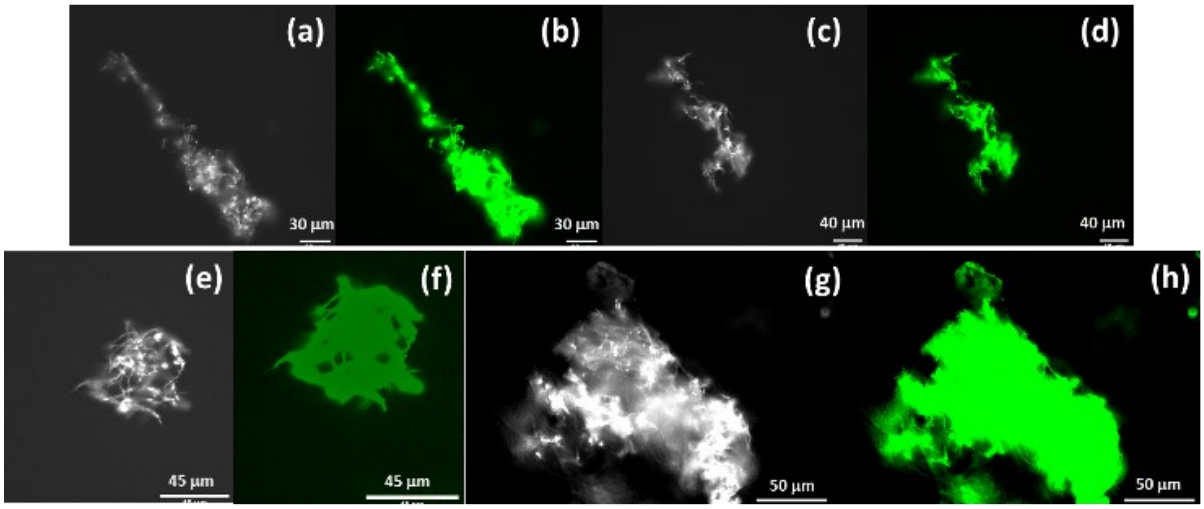

Fig. S1. Fluorescence microscopy images at the different stages of application of CTAB to the ct-DNA-bound 3-HF: (a, b) 0, (c, d) 30, (e, f) 150 and (g, h) 400 µM in aqueous buffered medium (pH 7.4). We have presented the non-colored images along with the colored ones for clarity.

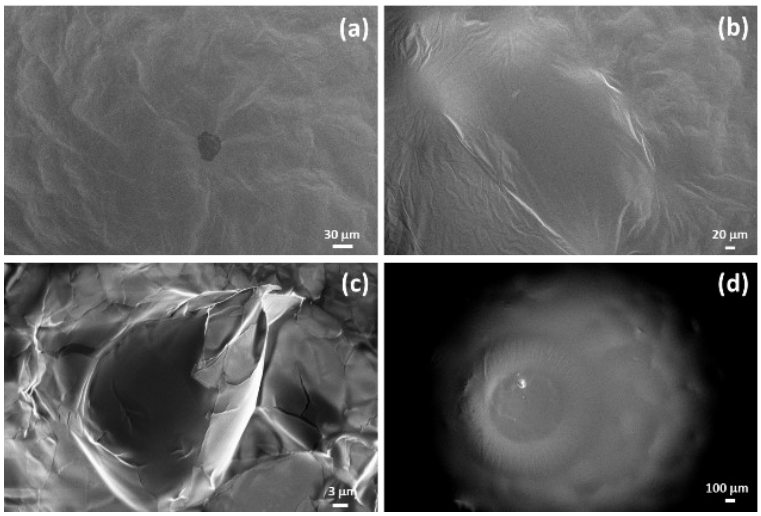

Fig. S2. SEM images at the different stages of application of CTAB to the ct-DNA: (a) 0, (b) 30, (c) 150 and (d) 400 µM in aqueous buffered medium (pH 7.4).

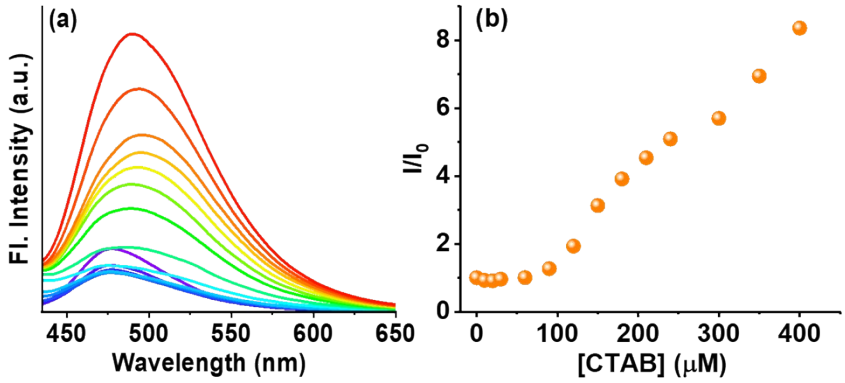

Fig. S3. (a) Fluorescence spectra of 3-HF bound to the minor groove of ct-DNA interacting with different concentrations of CTAB (0-400 μM), and (b) the relative change in the emission intensity (monitored at 510 nm) due to the interactions in neutral aqueous buffer medium (pH 7.4) at 22 °C. The samples were excited at 410 nm.

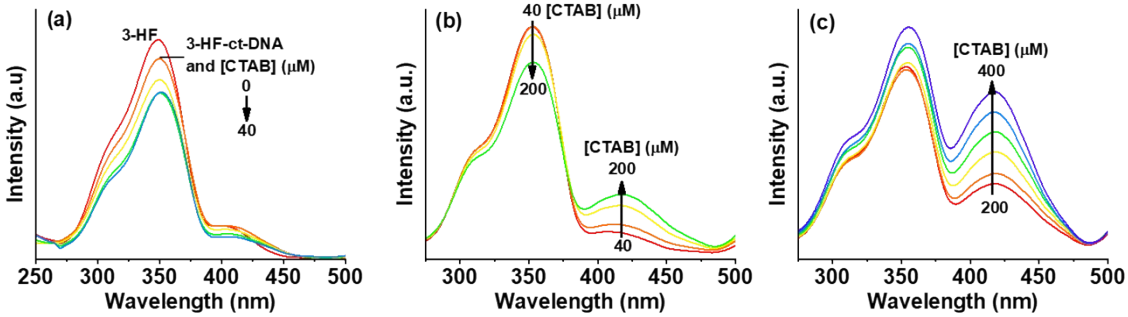

Fig. S4. The excitation spectra of 3-HF bound to ct-DNA on addition of various concentrations of CTAB (a) 0 to 40, (b) 40-200 and (c) 200-400 μM CTAB in aqueous buffer with pH 7.4 at 22 °C.

Table S1. Time-resolved fluorescence decay data of 3-HF on interaction with various concentrations of CTAB in aqueous medium. The samples were excited at 375 nm and the 510 nm emission was monitored. The τ's and the α's are the lifetimes and the percentage contributions to the fluorescence decay, respectively and the χ^2 values present the goodness of the fits. The data are within acceptable error limits.

[CTAB] (μM)	τ_1 (ps)	α_1	τ_2 (ps)	α_2	χ^2
0	178	86	860	14	1.24
30	232	74	1240	26	1.21
150	229	72	1150	28	1.33
400	704	55	188	45	1.43

Table S2. Time-resolved fluorescence decay data of ct-DNA-bound 3-HF on interaction with various concentrations of CTAB in aqueous medium. The samples were excited at 375 nm and the 510 nm emission was monitored. The τ's and the α's are the lifetimes and the percentage contributions to the fluorescence decay, respectively and the χ^2 values present the goodness of the fits. The data are within acceptable error limits.

[CTAB] (μM)	τ_1 (ps)	α_1	τ_2 (ps)	α_2	τ_3 (ps)	α_3	χ^2
0	9120	46	256	37	1230	17	1.2
30	9040	39	253	41	1110	20	1.18
150	1110	59	428	37	80	4	1.16