

Supporting Information

Unveiling the Self-Assembling Behavior of 5-Fluorouracil and its N,N'-Dimethyl Derivative : A Spectroscopic and Microscopic Approach

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1. Instrumentation.

1.1. Field Emission Scanning Electron Microscopy (FESEM) Measurements. FESEM measurements were executed with a Supra 40 (Carl Zeiss Pvt. Ltd) instrument after drop casting the sample on a glass slide and complete evaporation of the solvent.

1.2. Transmission Electron Microscopy (TEM) Measurements. Transmission electron microscopy (TEM) analysis was carried out by using JEOL model JEM 2010 transmission electron microscope at an operating voltage 200 kV. TEM samples were prepared by blotting a carbon coated (50 nm carbon film) Cu grid (300 mesh, electron microscopy science) with a drop of solution and the samples are allowed to be dried for overnight.

1.3. Fourier Transform Infrared Spectroscopy (FTIR): FTIR spectra of all samples were recorded in the range of 650–4000 cm^{-1} with a Nexus 870 FT-IR spectrometer using a ZnSe cell (MB/HATR Combo Kit Nexus). Each sample was recorded with 32 scans at a spectral resolution of 1.928 cm^{-1} . All the measurements were carried out at room temperature ($\sim 25^{\circ}\text{C}$). For each spectral deconvolution, using OMNIC software (version-6.0) of the Thermo Nicolet Corporation, we used the same bandwidth and enhancement.

2. Supporting Table.

Table S1 : Diffusion Parameters Obtained by Fitting the Fluorescence Correlation Curves of DCM in 5-FU Fibrils in Different pH of PBS.

compound	pH	τ (μs)	D_t ($\mu\text{m}^2 \text{s}^{-1}$)	R^2
5-FU (PBS)	5.6	172 ± 13	193 ± 14	0.92
	8.0	155 ± 10	214 ± 13	0.94

2. Supporting Figures.

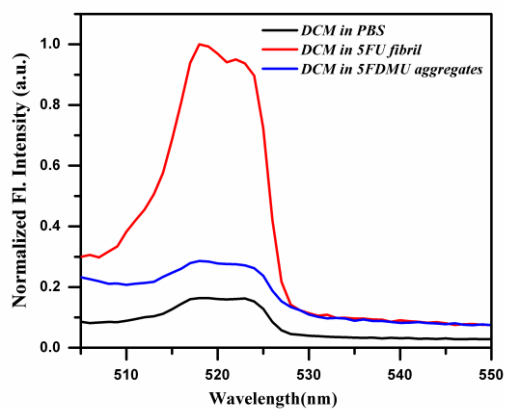


Figure S1 . Steady state emission spectra of DCM in 5-FU fibrils (red) and 5-FDMU aggregates (blue) with respect to blank (i.e. DCM in PBS only).

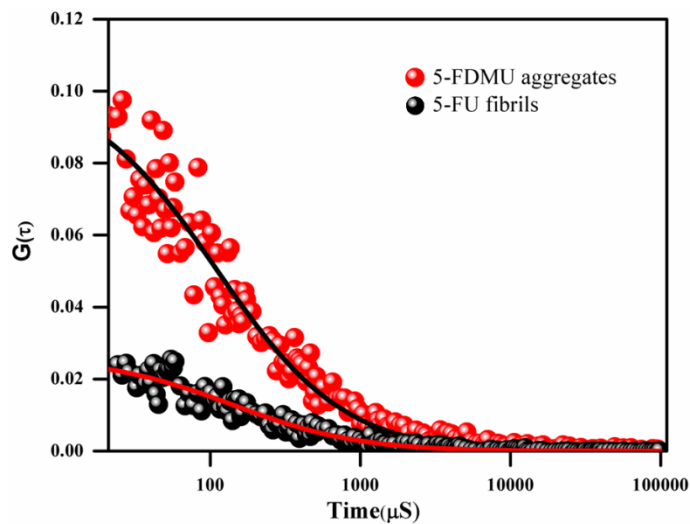


Figure S2 : FCS traces for 5-FU fibrils and 5-FDMU aggregates. The solid lines indicate fitted to the data point.

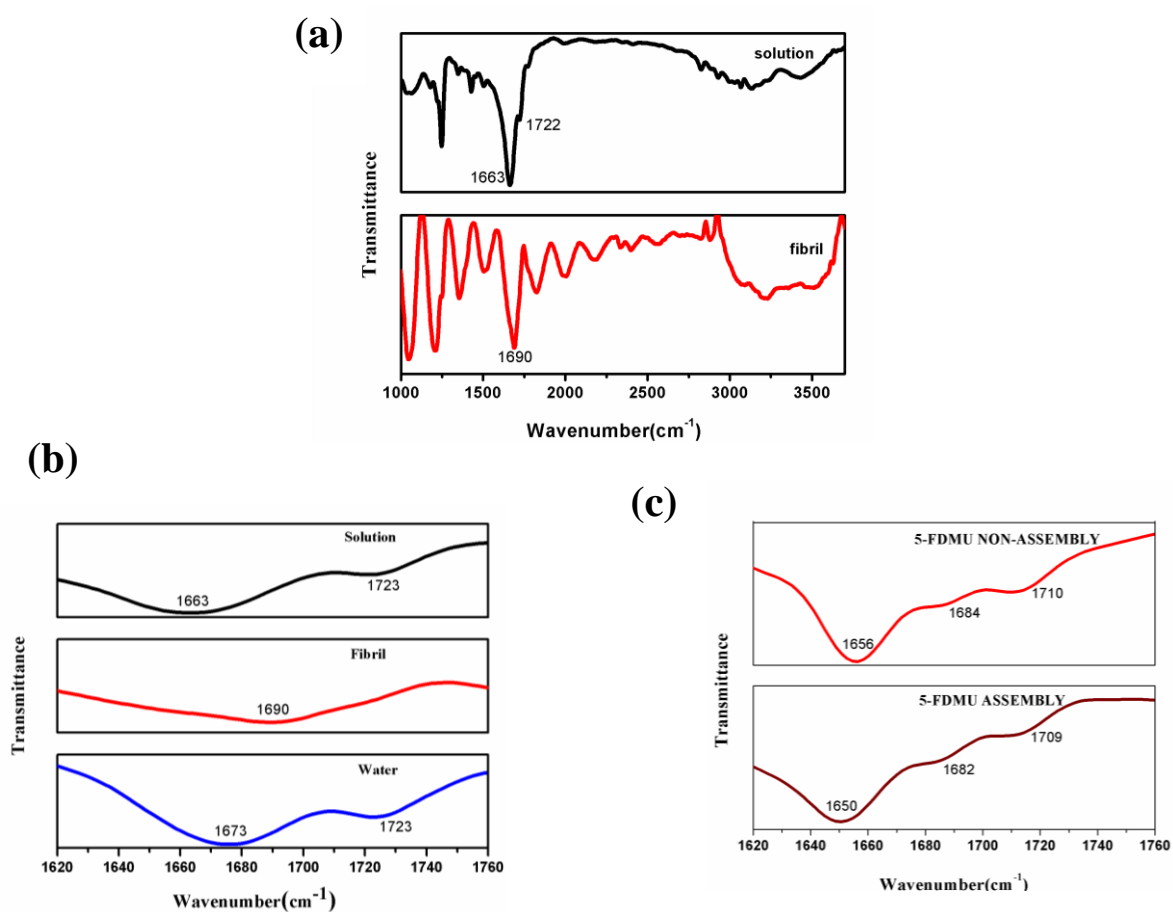


Figure S3 . FTIR spectra of (a) 5-FU initial solution and fibrillar solution in PBS (b) Monitoring carbonyl peaks of 5-FU in initial solution in PBS, fibrillar solution in PBS and water solution (c) 5-FDMU carbonyl peaks in non-assembly and assembly conditions in PBS.

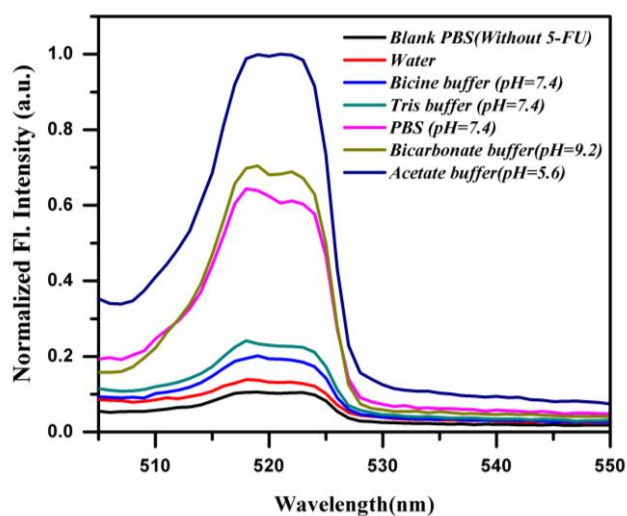


Figure S4 : Steady state emission spectra of DCM in 5-FU fibrils/aggregates in different buffers.

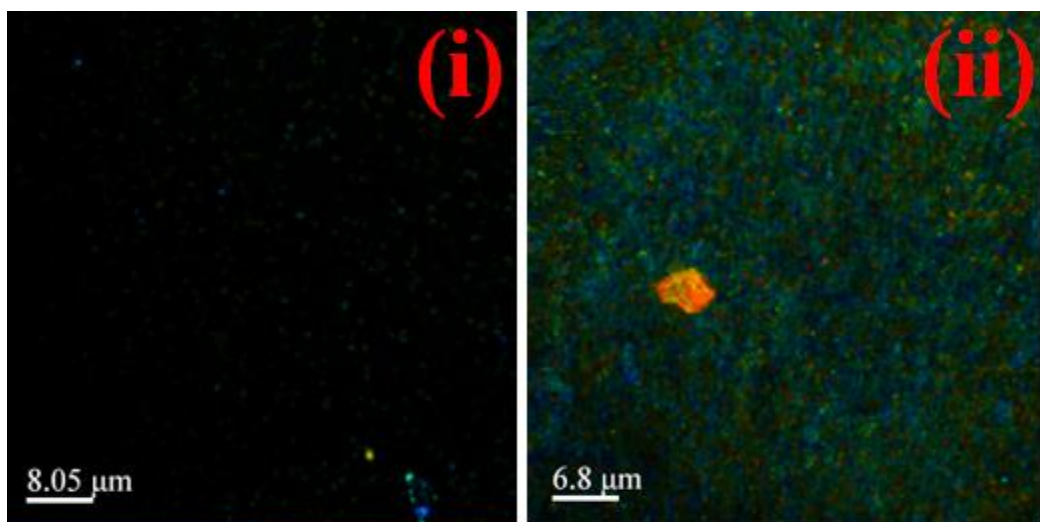


Figure S5: FLIM images DCM in 100 mM (i) PBS (scale bar is 8.05 μm) (ii) Tris buffer (scale bar is 6.8 μm).

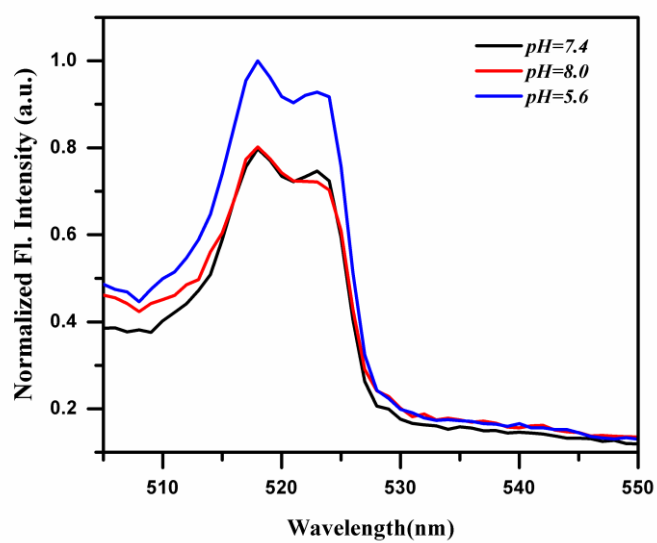


Figure S6. Normalized Steady state emission spectra of DCM in 5-FU fibrils at three different pH of PBS.