Supporting Information

Interaction of a Julolidine-Based Neutral Ultrafast Molecular Rotor with Natural DNA: Spectroscopic and Molecular Docking Studies

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Ground-state absorption studies of aqueous solution of DCVJ: Due to low solubility in water, the addition of highly concentrated methanolic solution of DCVJ into water may result in the formation of aggregates. To check such possibility, we have recorded the absorbance of aqueous solution of DCVJ at different concentrations and results are shown in Figure S1. Absorbance of DCVJ varies linearly with the concentration till $8x10^{-6}$ mol dm^{-3} and shows negative deviation beyond $8x10^{-6}$ mol dm^{-3} indicating the onset of aggregation. This experiment confirms that DCVJ present as monomer in the experimental solution ($1.8x10^{-6}$ mol dm^{-3})

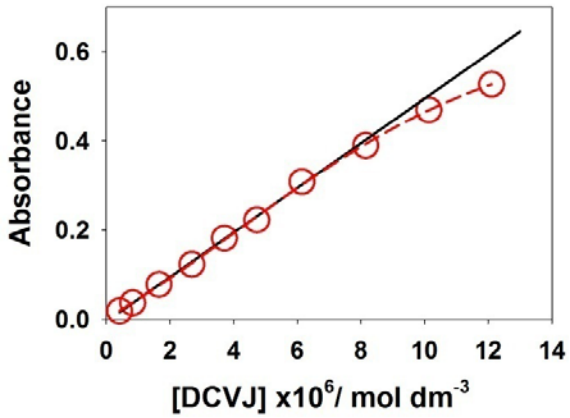


Figure S1. Variation in the absorbance of DCVJ with concentration in aqueous solution.

Optical microscopic studies with aqueous solution of DCVJ: To further check the formation of aggregates due to the addition of concentrated methanolic solution of DCVJ into water, microscopic images have been recorded for aqueous solutions of DCVJ at different concentrations. Images have been recorded using Olympus microscope (Model BX53). For imaging studies, solutions are prepared by adding requisite amount of DCVJ in methanol to water and images were recorded on glass slides. Microscopic images of aqueous DCVJ solution of 1.8 and $12x10^{-6}$ mol dm^{-3} are shown in Figure S2. It is evident from this figure that microscopic aggregates are formed in $12x10^{-6}$ mol dm^{-3} solution and but no such formation of aggregates are observed in $1.8x10^{-6}$ mol dm^{-3} solution. This result is in agreement with the absorption studies (cf. Figure S1). Hence, our studies show that DCVJ exist as monomer in the experimental solution ($1.8x10^{-6}$ mol dm^{-3})

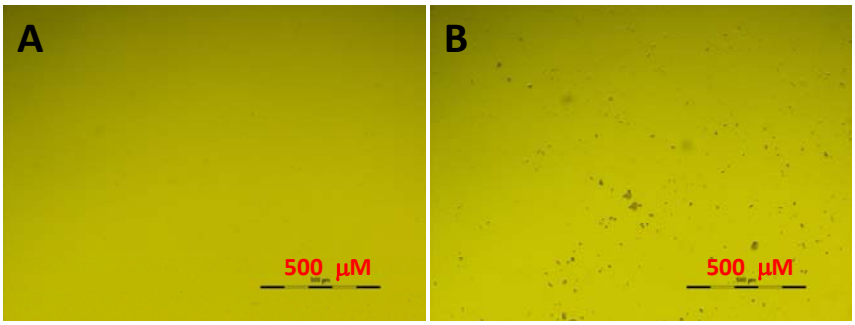


Figure S2. Optical microscopic images of aqueous solution of (A) $1.8x10^{-6}$ mol dm^{-3} and (B) $12x10^{-6}$ mol dm^{-3} DCVJ.

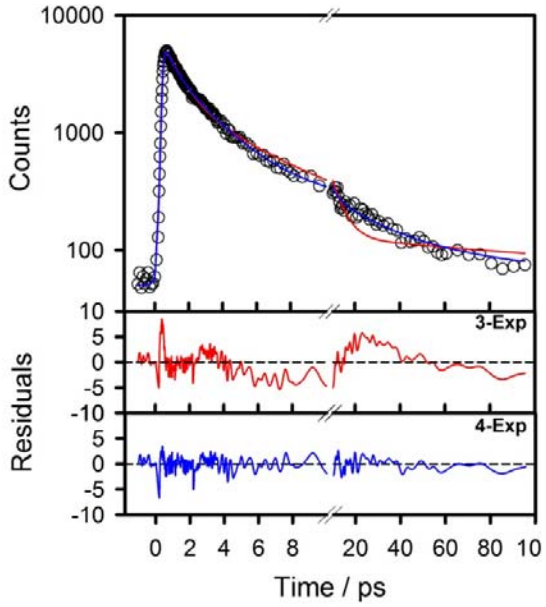


Figure S3. Fitting of the transient emission decays for DCVJ in $4x10^{-3}$ mol dm^{-3} DNA in the presence of 0.5 mol dm^{-3} NaCl by triexponential (red solid line) and tetraexponential (blue solid line) decay functions. Residuals for each fitting are shown in the lower panels.

Effect of salt on emission of DCVJ: The effect of salt on the emission of DCVJ in pure water has also been investigated and the results are shown in Figure S4. It is evident from the figure that added salt does not have much effect on the emission of DCVJ in pure water. However, a marginal increase in the emission intensity of DCVJ takes place due to addition of 0.5 mol dm^{-3} NaCl. Such marginal increase in the emission intensity might be due to the nominal increase in the viscosity of the aqueous solution due to addition of salt. For example, Kestin et al.(J. Phys. Chem. Ref. Data, 1981, 10, 71-87) have shown that the viscosity of water at 25 ^{O}C changes from 0.89 cP to 0.93 cP due to addition of 0.5 mol dm^{-3} NaCl. Hence, the observed substantial decrease in the emission intensity of DCVJ in DNA solution upon addition of salt, as mentioned in the main text, is not due to direct interaction between free DCVJ and salt, rather, it is due to the changes in the binding force between DCVJ and DNA upon addition of salt.

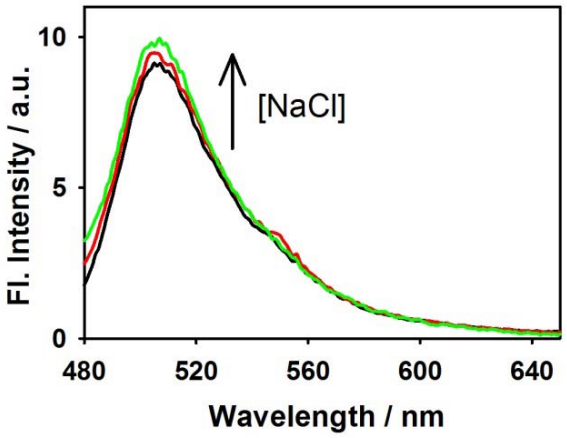
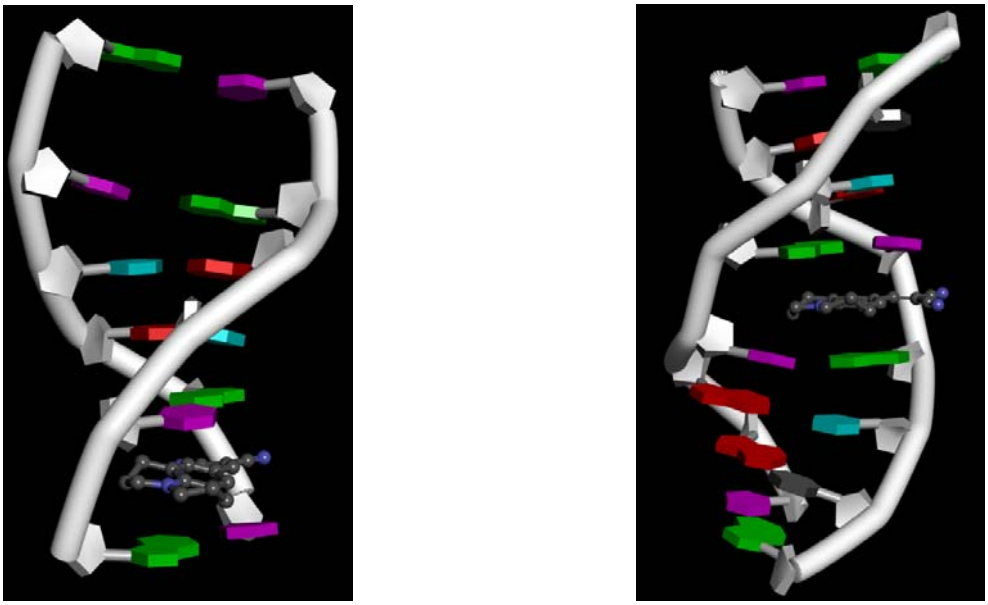


Figure S4. Emission spectra of aqueous solution of DCVJ in the presence of different concentrations of NaCl (0-0.5 mol dm^{-3}).

Docking with additional DNA molecules: Molecular docking of DCVJ with short DNA molecules having different sequences and sizes have also been studied. Two DNA molecules with sequence, CGATCG and GUTGCAAC having pdb ID of 1Z3F and 454D, respectively, have been used for the molecular docking and the results are shown in the Figure S5. It is evident from these two docked configurations of DCVJ-DNA complex that irrespective of the sequence and size of the DNA, DCVJ interact with DNA mainly by intercalative modes.



1Z3F 454D

Figure S5. Docked configuration of DCVJ with two different DNA molecules.