Supporting Information

Fluorescence Probing of Aminofluorene-induced Conformational Heterogeneity in DNA Duplexes

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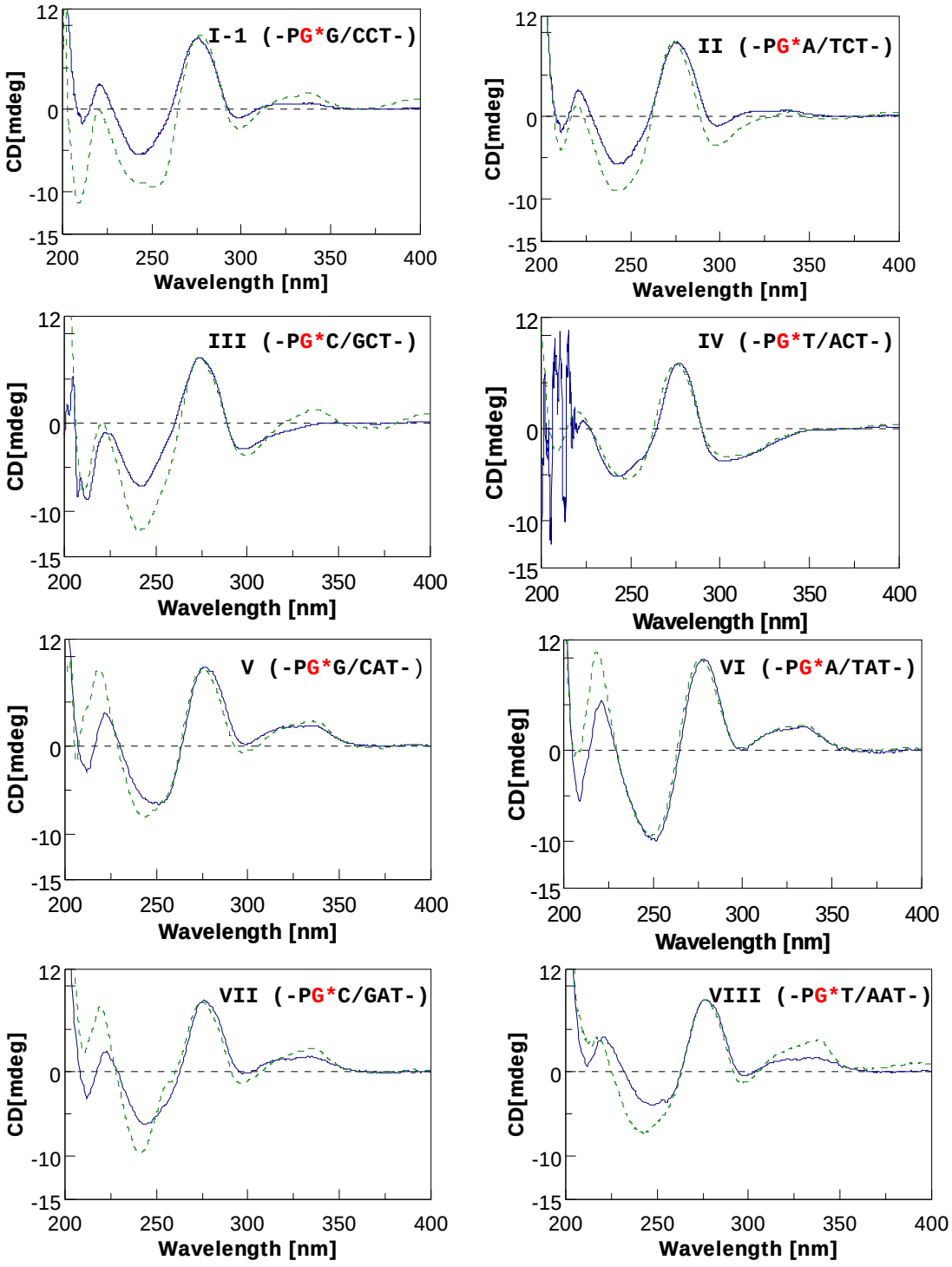


Figure S1: Normalized CD overlays of the FAF modified AP (solid blue) and A (dotted green) containing duplexes I-VIII

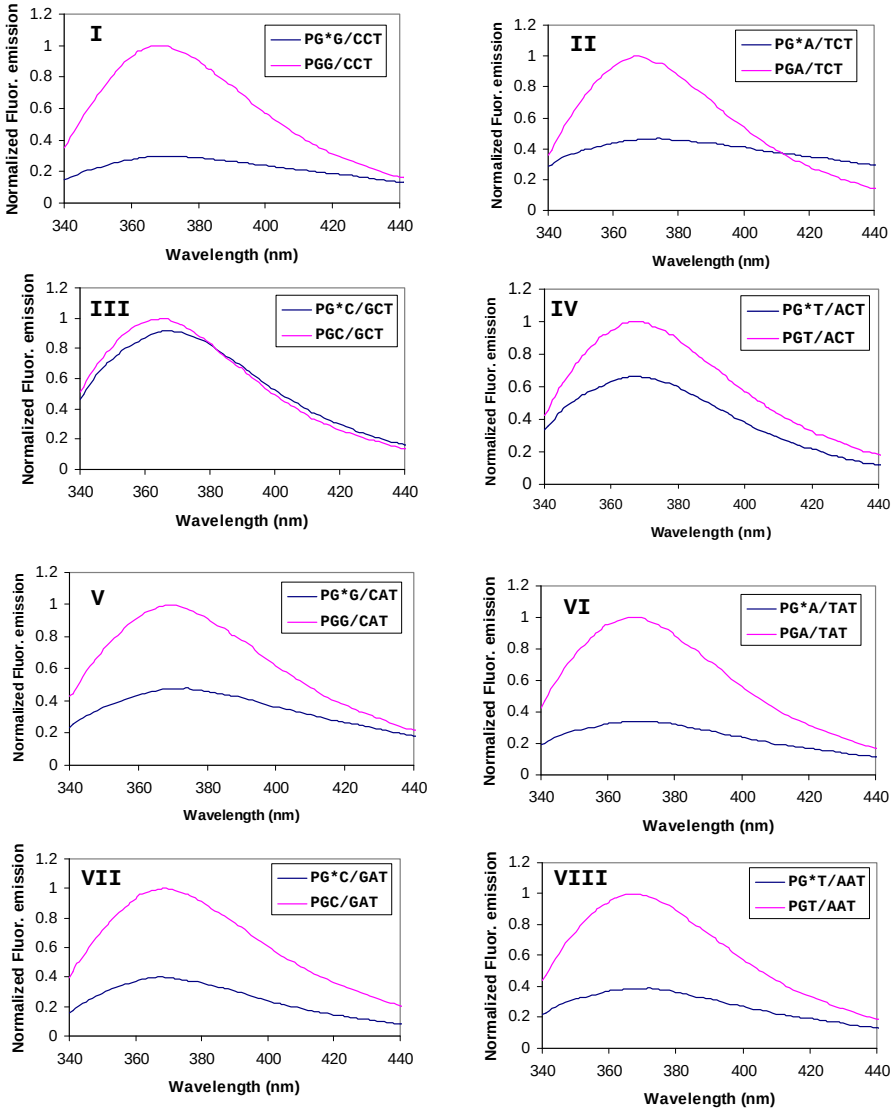


Figure S2: Normalized fluorescence emission spectra (λ_{ex} = 310 nm) of the unmodified control (pink) and FAF-modified (blue) duplexes (I-VIII) (15μM) in 10 mM sodium phosphate at pH 7. Fluorescence emissions of FAF-modified duplexes (I, II) and (V, VI, and VIII) are red-shifted by 6 and 4 nm, respectively, relative to the controls.

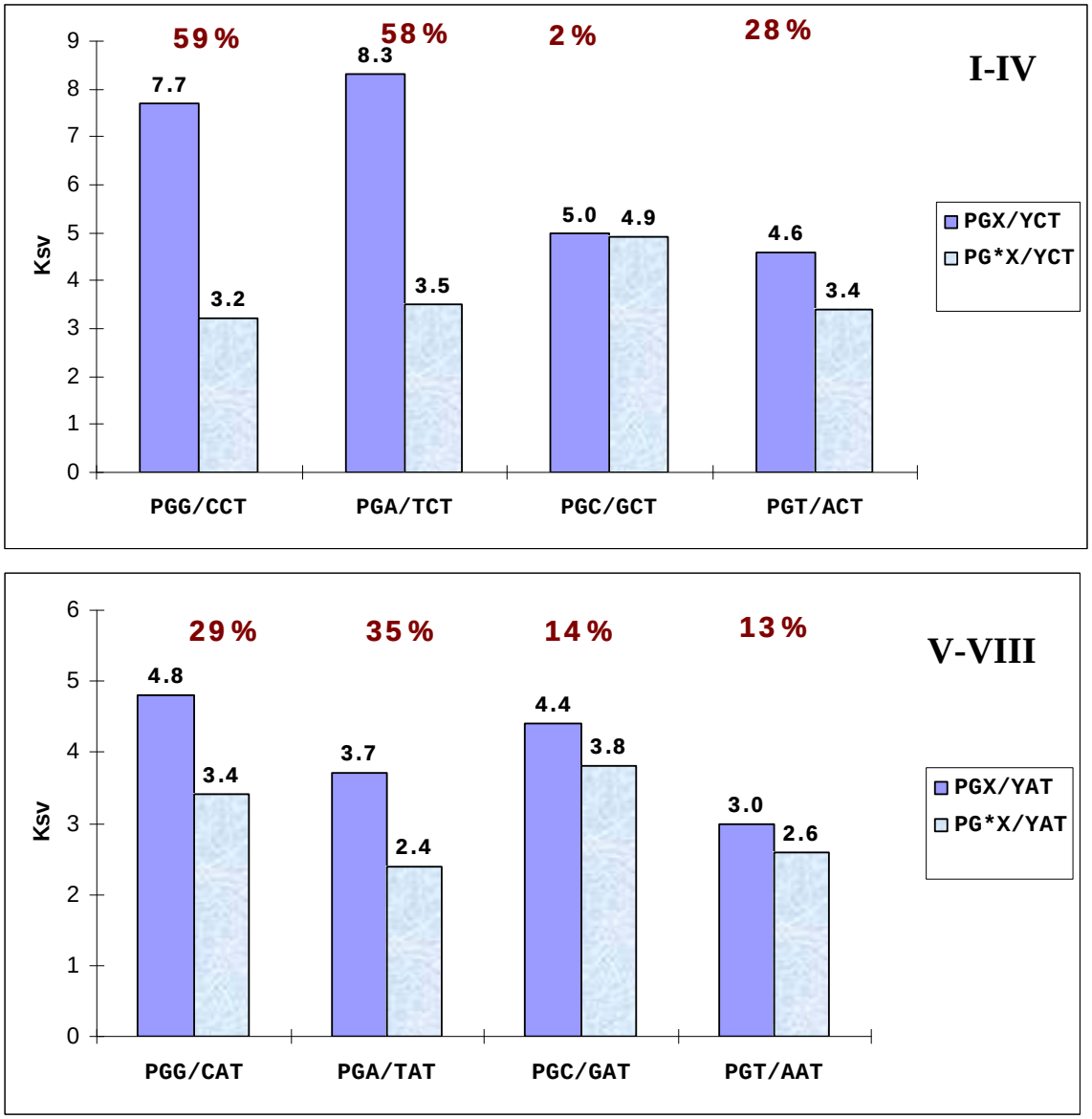
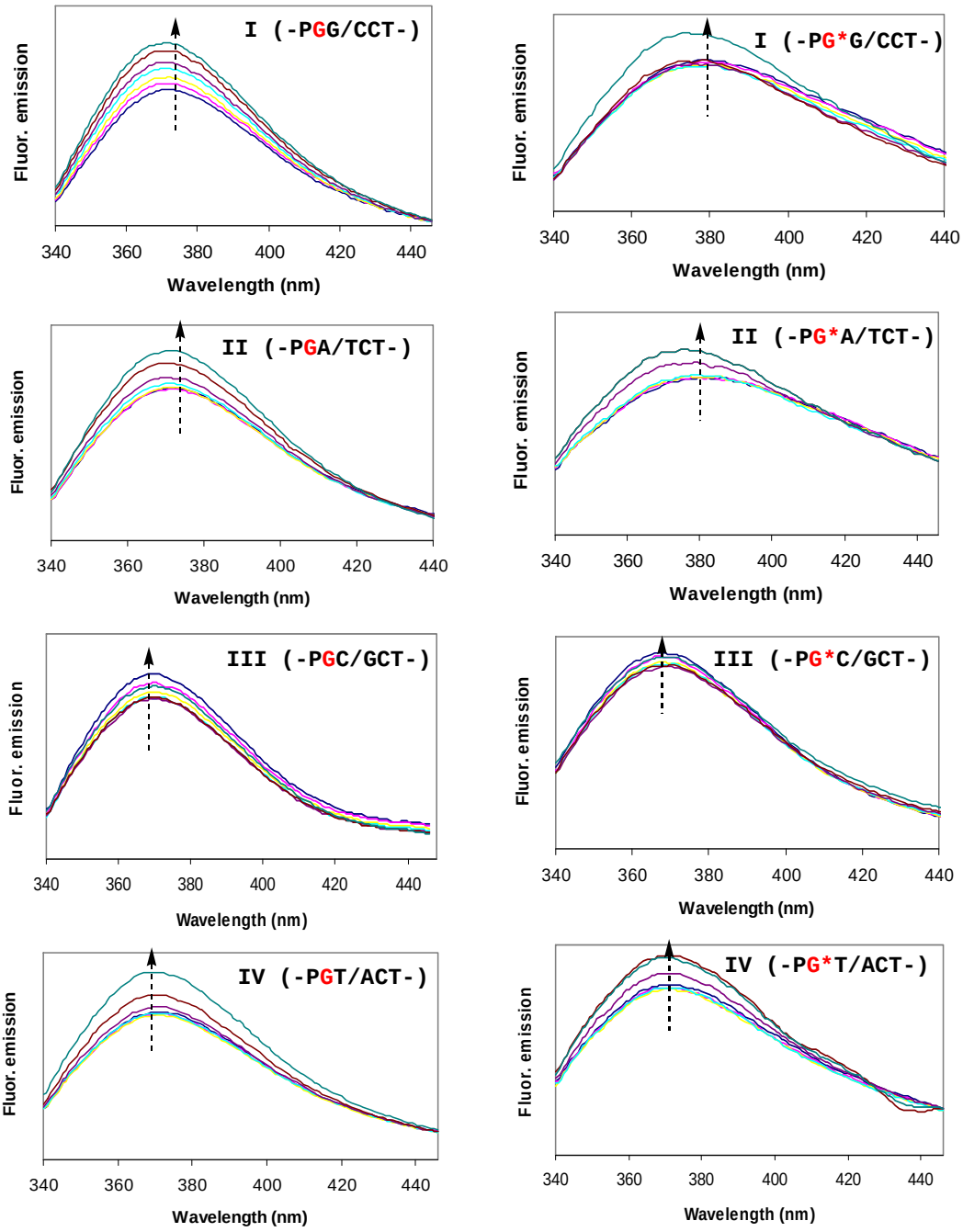


Figure S3: Stern-Volmer constant (*Ksv*) for the unmodified control (blue) and FAF-modified (cyan) duplexes (I-VIII) derived from acrylamide experiments. The numbers on top of the bar graph refer to % reduction of *Ksv* for each duplex upon adduct formation (X, Y = G, A, C, T).

(A) **Control** **Modified**



(B) **Control** **Modified**

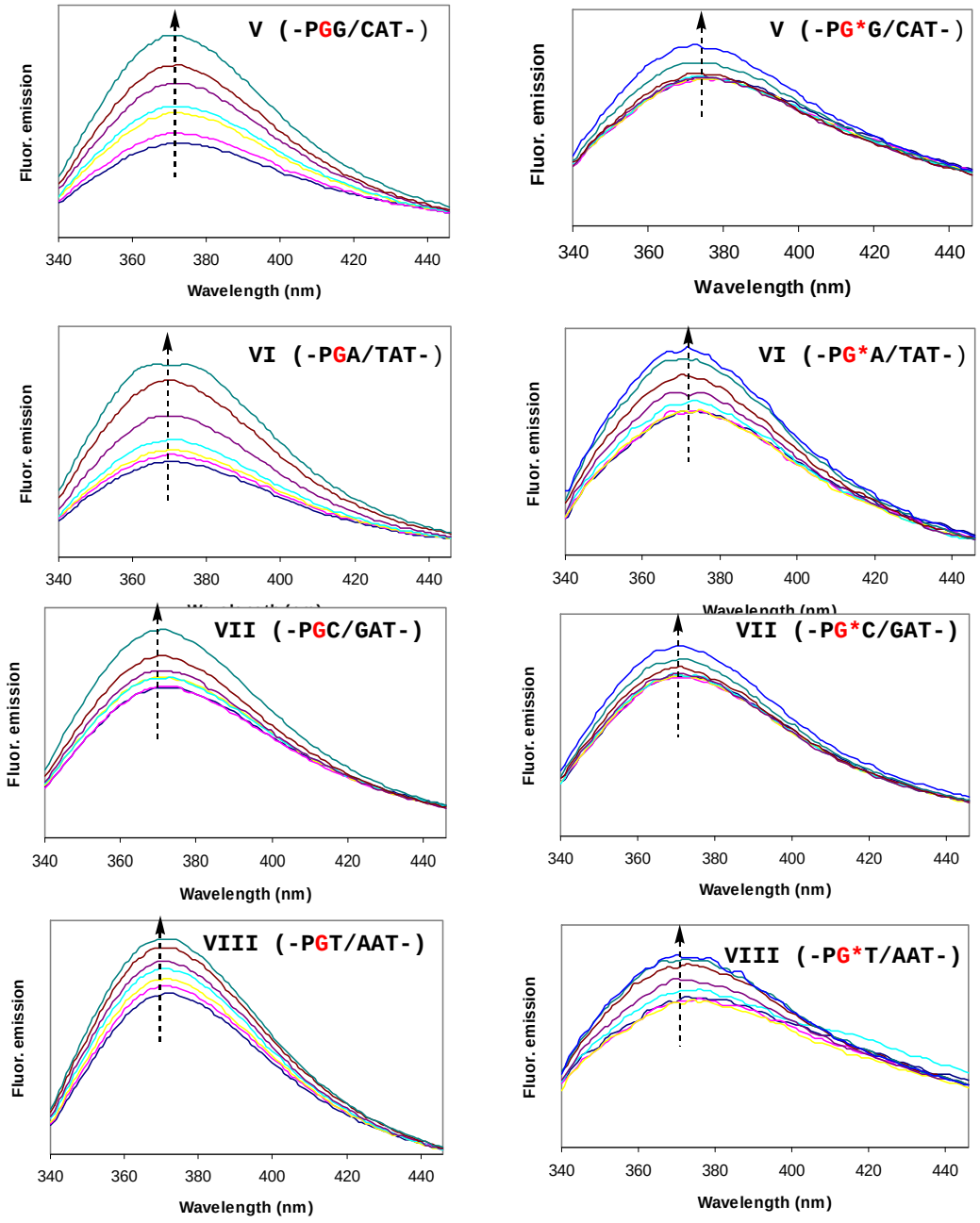


Figure S4: (A) Fluorescence emission spectra of FAF modified and unmodified duplexes I-IV as a function of temperature from 5-45ºC. Fluorescence intensity for the control duplexes increased steadily with temperature. The fluorescence intensity of FAF modified ODNs in this study remained constant until the temperature rose above 40ºC and then began to increase sharply as Tm approached. (B) Fluorescence emission spectra of the FAF-modified and unmodified duplexes V-VIII as a function of temperature from 5-45ºC.

Table S1: Calculated and measured molecular weights (m/z) for the FAF-modified 12-mer ODNs used in this study.

Sample	Sequence	Calculated Mass	Measured Mass
ODN I-1	CTTCTPG(FAF)GCCTC	3767.7	3767.6
ODN I-2	CTTCTPGG(FAF)CCTC	3767.7	3767.8
ODN II	CTTCTPG(FAF)ACCTC	3751.7	3751.7
ODN III	CTTCTPG(FAF)CCCTC	3727.7	3727.7
ODN IV	CTTCTPG(FAF)TCCTC	3742.7	3742.8