

Investigations on self-structure formation in polyadenylic acid by planar dyes: Comparative spectroscopic and calorimetric studies of thionine and toluidine blue O

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Supplementary Data

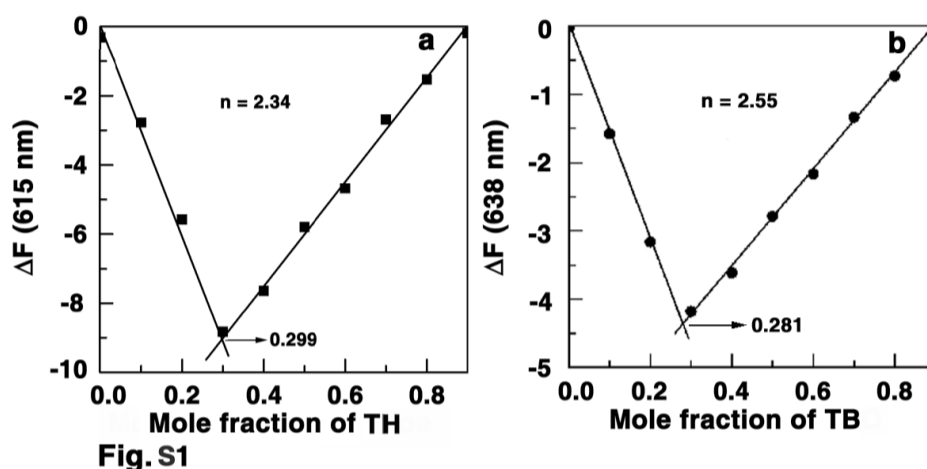


Fig. S1. Job plot for the binding of (a) TH (■) and (b) TB (●) to ss poly(A).

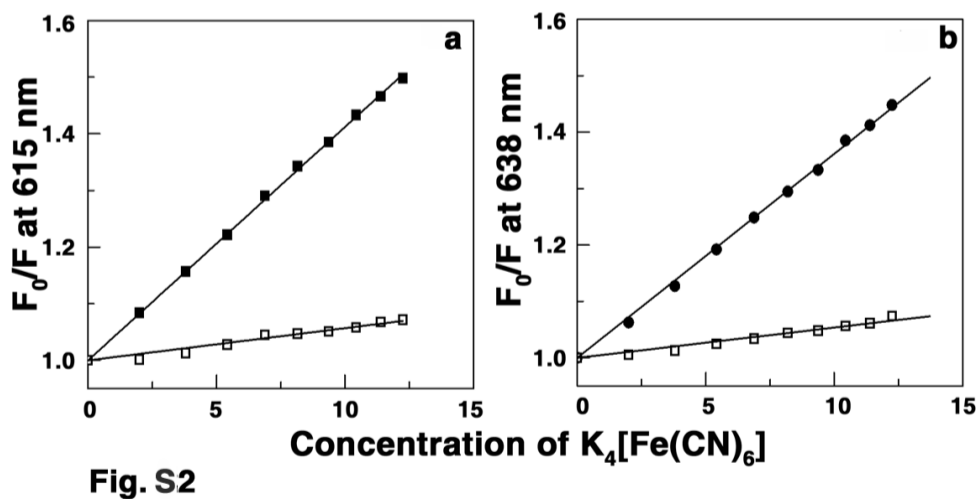


Fig. S2. Stern-Volmer plots for the quenching of (a) TH (■) and (b) TB (●) and complexes of TH- ss poly(A) (□) and TB- ss poly(A) (○) with increasing concentration of $K_4[Fe(CN)_6]$.

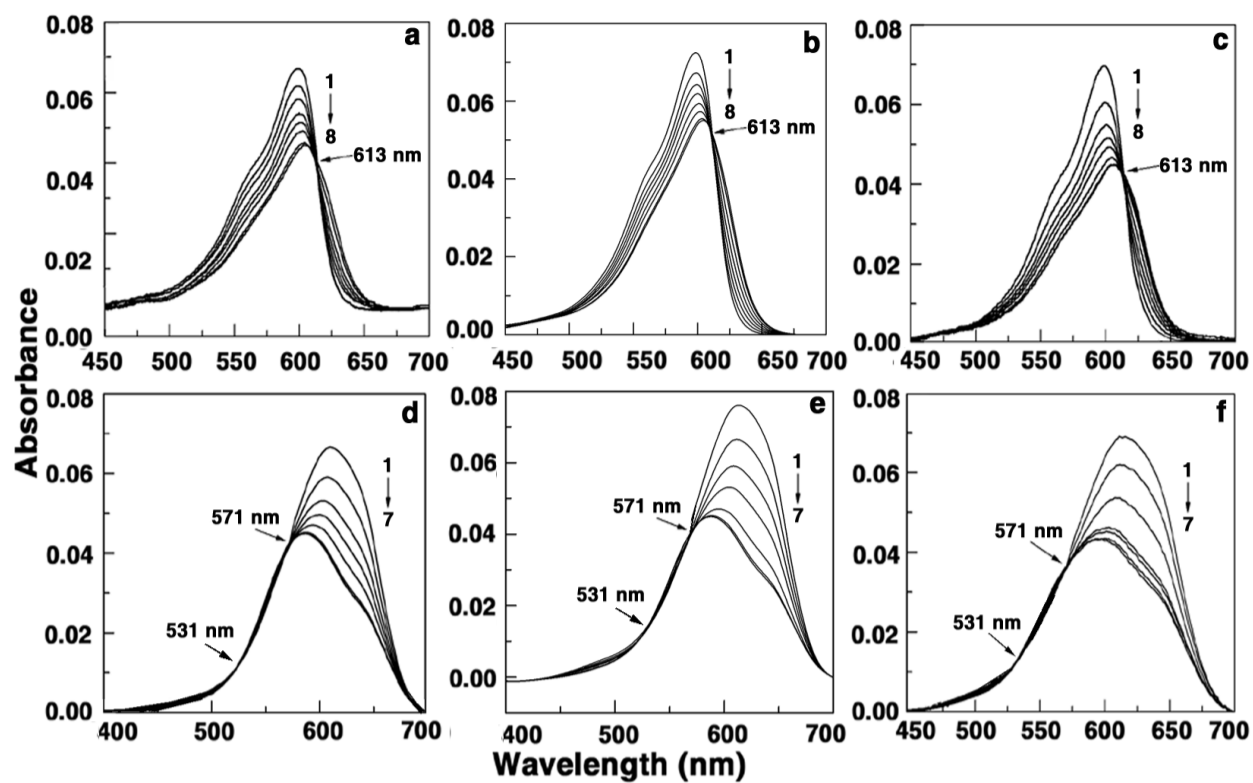


Fig. S3

Fig. S3. Absorbance titration of TH (upper panels) and TB (lower panels) in (a,d) 50 mM, (b,e) 100 mM and (c,f) 200 mM $[\text{Na}^+]$ concentrations.

Table S1: Summary of the optical properties of free and ss poly (A) bound dyes^a.

Parameter	TH	TB
Absorbance		
λ_{\max} (free)	598	618
λ_{\max} (bound)	606	587
λ_{iso} ^b	613	531, 571
ϵ_f (at λ_{\max})	54,200	29,200
ϵ_b (at λ_{\max})	40,390 (598)	14,270 (618)
ϵ_{iso} (at λ_{iso})	39,428 (613)	14,123 (571)
Fluorescence		
λ_{\max} (excitation)	596	620
λ_{\max} (emission)	615	638

^aUnits: λ (wavelength) nm; ϵ (molar extinction coefficient) $\text{M}^{-1} \text{cm}^{-1}$. ^bWavelengths at the isosbestic points.

Table S2: Binding parameters for the complexation of the two dyes with ss poly(A) evaluated from Scatchard analysis of the absorbance titration data^a.

Dyes studied	Salt	$K \times 10^{-5} \text{ (M}^{-1}\text{)}^b$	n	ω	$K \times 10^{-6} \text{ (M}^{-1}\text{)}^b$
TH	50	2.66±0.02	2.23	20	5.32±0.02
	100	3.21±0.04	2.21	25	8.02±0.04
	200	3.11±0.03	2.19	29	9.02±0.03
TB	50	0.67±0.03	2.58	60	4.02±0.03
	100	0.99±0.01	2.51	71	7.03±0.01
	200	1.11±0.02	2.44	75	8.33±0.02

^aAverage of four determinations. ^bBinding constants (K) and the number of binding sites (n) conducted in sodium cacodylate buffer of (50, 100 and 200) mM $[\text{Na}^+]$, pH 7.2. ω is the cooperativity factor.