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Electronic Supplementary Information

Probing the interaction of spermine and 1-naphthyl acetyl spermine with DNA polynucleotides: A comparative biophysical and thermodynamic investigation

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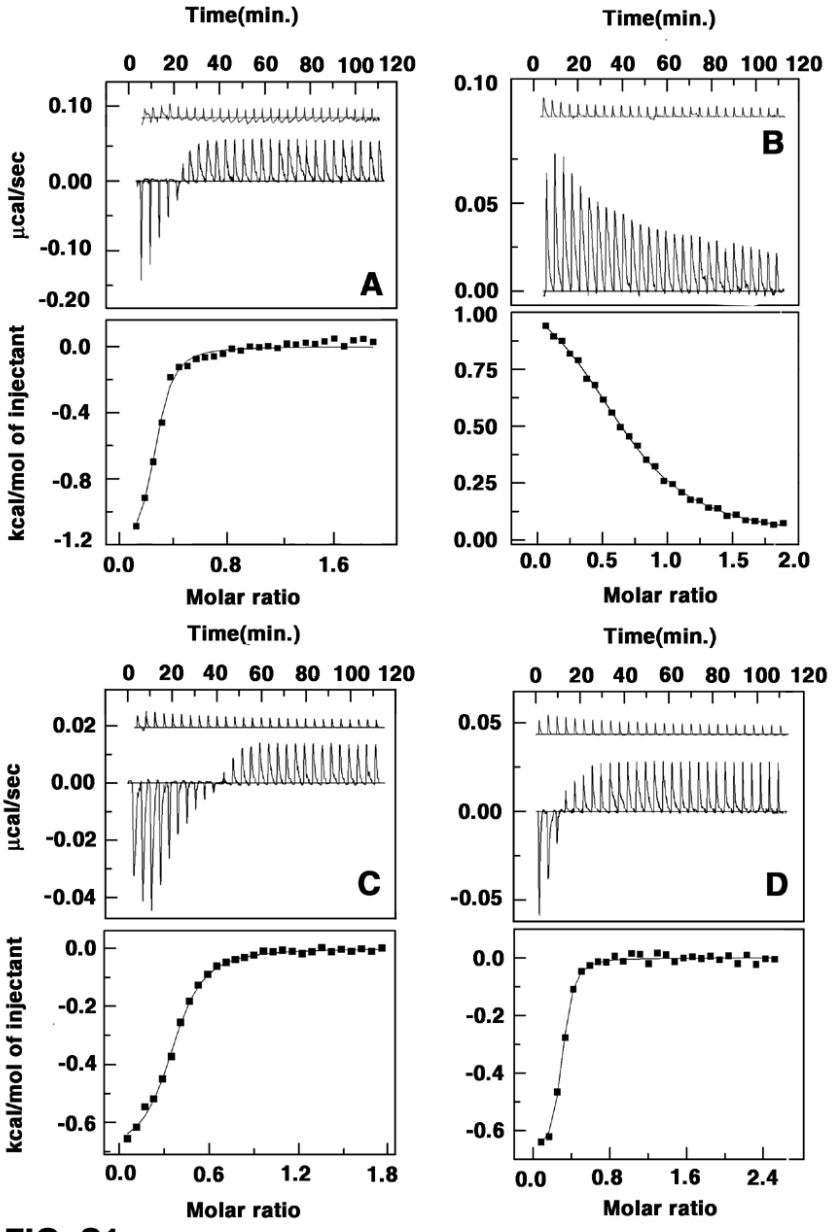

FIG. S1

Fig. S1. ITC profiles for the titration of SPM with (A) poly(dG).poly(dC) (B) poly(dG-dC).poly(dG-dC) and titration of NASPM with (C) poly(dG).poly(dC) (D) poly(dG-dC).poly(dG-dC). The top panels represent the raw data for the sequential injection of SPM and NAPSM into a solution of DNA polynucleotide and the bottom panels show the integrated heat data after correction of heat of dilution against molar ratio of DNA polynucleotide/[polyamine]. The data points were fitted to one site model and the solid line represent the best fit data.

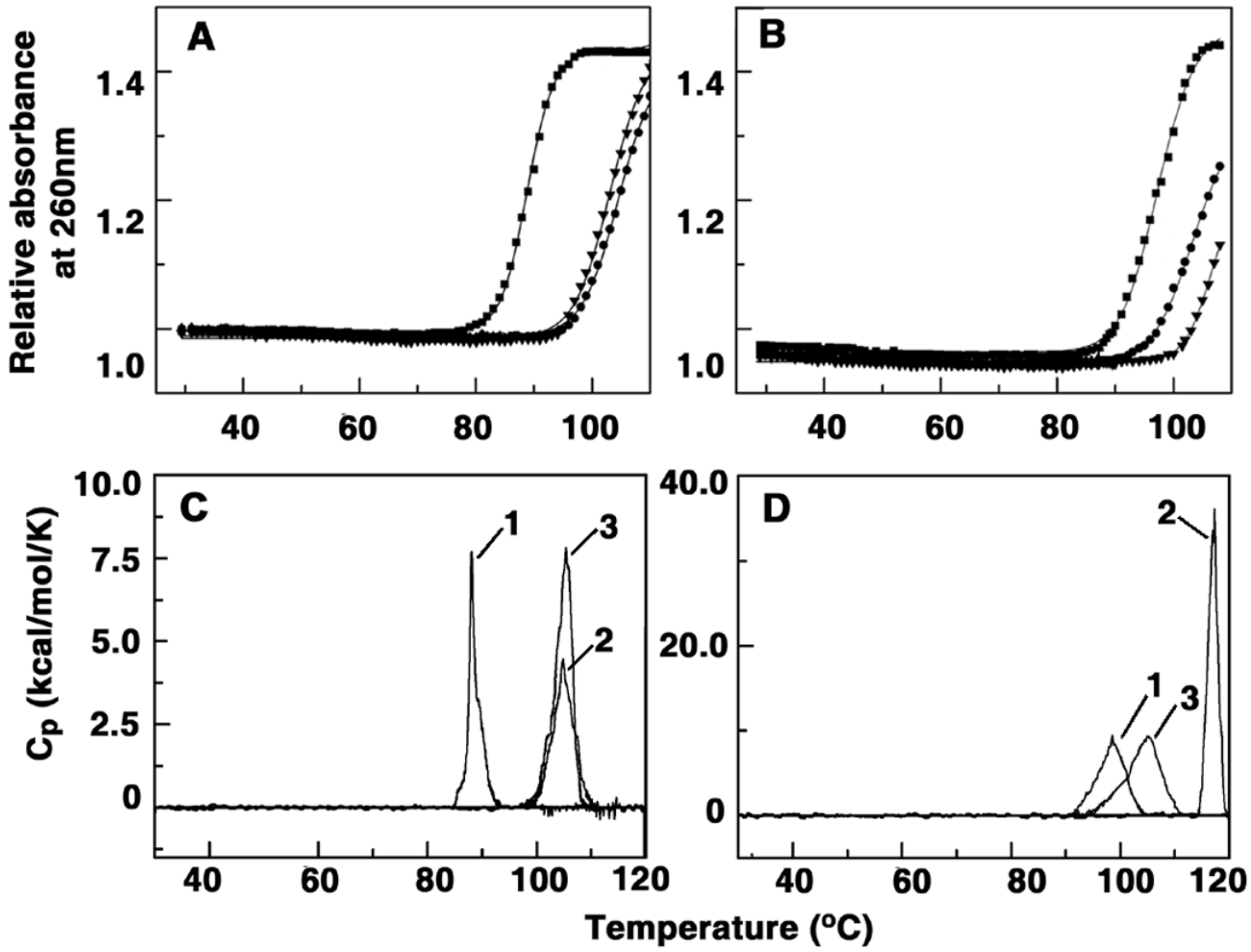

FIG. S2

Fig. S2. Optical melting profiles (lower panels) (A) poly(dG).poly(dC) (O), NASPM complex (❑), SPM complex (ஜ), (B) poly(dG-dC).poly(dG-dC) (O), NASPM complex (❑), SPM complex (ஜ).. DSC melting profiles (upper panels) of (C) poly(dG).poly(dC) (curve1), NASPM complex (curve 2), SPM complex (curve 3), (D) poly(dG-dC).poly(dG-dC) (curve1), NASPM complex (curve 2), SPM complex (curve 3)..

Table S1: ITC derived thermodynamic parameters for the binding of SPM and NASPM to poly(dG).poly(dC) and poly(dG-dC).poly(dG-dC). [a]							
Polyamines	Temperature (K)	K ($\times 10^5$ M^{-1})	N	$\Delta G°$ (kcal/mol)	$\Delta H°$ (kcal/mol)	$T\Delta S°$ (kcal/mol)	$\Delta C_p{}^o$ (cal/mol K)
Poly(dG).poly(dC)							
SPM	283.15	11.1±0.17	0.294±0.003	-7.816±0.019	-0.656±0.009	7.160±0.012	-60.6±0.01
	288.15	8.33±0.07	0.278±0.003	-7.824±0.021	-0.912±0.011	6.912±0.016	
	293.15	6.63±0.13	0.252±0.008	-7.796±0.013	-1.262±0.006	6.534±0.020	
NASPM	283.15	6.80±0.07	0.404±0.004	-7.561±0.012	-0.175±0.003	7.386±0.011	-52.9±0.11
	288.15	5.23±0.06	0.372±0.006	-7.537±0.018	-0.337±0.007	7.200±0.016	
	293.15	3.93±0.03	0.357±0.004	-7.502±0.021	-0.704±0.011	6.798±0.013	
Poly(dG-dC).poly(dG-dC)							
SPM	283.15	1.71±0.08	0.703±0.005	-6.782±0.011	1.708±0.018	8.491±0.013	-52.7±0.03
	288.15	0.93±0.01	0.699±0.009	-6.546±0.013	1.403±0.027	7.949±0.020	
	293.15	0.74±0.01	0.696±0.007	-6.525±0.017	1.181±0.016	7.706±0.013	
NASPM	283.15	13.3±0.37	0.358±0.003	-7.931±0.015	-0.092±0.014	7.839±0.014	-78.7±0.01
	288.15	10.5±0.10	0.283±0.001	-7.984±0.021	-0.409±0.002	7.574±0.021	
	293.15	8.83±0.20	0.269±0.005	-7.969±0.019	-0.879±0.015	7.091±0.026	

[a]All the data in this table are derived from ITC experiments conducted in 20 mM [Na^+] citrate-phosphate buffer, pH 7.0 and are average of four determinations, K and ΔH^o values were determined from ITC profiles fitting to Origin 7 software as described in the text. The values of ΔG^o and $T\Delta S^o$ were determined using the equation $\Delta G^o = -RT\ln K$, and $T\Delta S^o = \Delta H^o - \Delta G^o$. All the ITC were fit to a model of single binding sites.

Table S2: ITC derived thermodynamic parameters for the binding of SPM and NASPM to poly(dG).poly(dC) and poly(dG-dC).poly(dG-dC) in CP buffer pH 7 at 20ºC at different [Na^+] concentration.[a]

Polyamines	[Na^+] mM	K ($\times 10^5\ M^{-1}$)	N	$\Delta G°$ (kcal/mol)	$\Delta H°$ (kcal/mol)	$T\Delta S°$ (kcal/mol)	$\Delta G°_{pe}$ (kcal/mol)	$\Delta G°_{t}$ (kcal/mol)
Poly(dG).poly(dC)								
SPM	10	15.2±0.13	0.438±0.003	-8.341±0.034	-1.929±0.017	6.412 ±0.025	-3.427±0.025	-4.914±0.036
	20	6.63±0.13	0.252±0.008	-7.855±0.054	-1.262±0.006	6.593±0.054	-2.911±0.040	-4.944±0.049
	30	3.97±0.32	0.196±0.003	-7.521±0.023	-0.748±0.017	6.773±0.012	-2.610±0.055	-4.911±0.027
NASPM	10	6.24±0.55	0.477±0.004	-7.820±0.052	-0.752±0.008	7.068±0.052	-3.778±0.062	-4.041±0.044
	20	3.93±0.03	0.357±0.004	-7.549±0.059	-0.704±0.011	6.845±0.059	-3.209±0.023	-4.339±0.035
	30	1.23±0.20	0.191±0.160	-6.868±0.063	-0.296±0.030	6.572±0.056	-2.876±0.078	-3.991±0.010
Poly(dG-dC).poly(dG-dC)								
SPM	10	1.29±0.08	0.703±0.008	-6.896±0.046	1.334±0.019	8.229±0.041	-2.780±0.058	-4.116±0.020
	20	0.74±0.01	0.696±0.007	-6.573±0.057	1.181±0.016	7.754±0.032	-2.361±0.021	-4.212±0.066
	30	0.40±0.03	0.381±0.017	-6.213±0.056	0.704±0.004	6.917±0.021	-2.116±0.048	-4.100±0.024
NASPM	10	15.4±0.16	0.308±0.002	-8.349±0.045	-1.120±0.013	7.229±0.033	-2.617±0.054	-5.731±0.022
	20	8.83±0.20	0.269±0.005	-8.021±0.040	-0.879±0.015	7.142±0.041	-2.223±0.049	-5.797±0.039
	30	5.44±0.01	0.258±0.005	-7.739±0.027	-0.431±0.011	7.308±0.028	-1.993±0.021	-5.745±0.021

[a]All data in this table are derived from ITC experiments conducted in citrate-phosphate buffer pH 7.0, and are an average of four determinations. K and ΔH^o values were determined from ITC profiles fitting to Origin 7 software as described in text. The values of ΔG^o and $T\Delta S^o$ were determined using the equations, $\Delta G^o = - RT\ln K$, and $T\Delta S^o = \Delta H^o - \Delta G^o$. All the ITC were fit to a model of single binding sites.