

Supplementary Information

Multimodal Investigation of Dacomitinib-Calf Thymus DNA Binding Interaction: Insights from Spectroscopy, Thermodynamics, and In-Silico Studies

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Table S1: Raw data for UV-Vis spectra of DCN-ctDNA complex using 5 increasing concentration of DCN and a fixed concentration of ctDNA (30.0 μM)

DCN Concentration (μM)	Absorbance ^a (at 260 nm)
0	0.18
2.1	0.23
4.2	0.28
6.3	0.33
8.4	0.38
10.5	0.43

^a Mean of three different determinations.

Table S2: Raw data for the effect of variable concentrations of DCN (0 – 10.5 μM) on the viscosity of ctDNA (30.0 μM) in Tris-HCl buffer

t_0^a (Sec)	t^a (Sec)	$t-t_0$	$t-t_0/t_0$	η_0 DNA	t^a Drug (Sec)	t_0^a DNA (Sec)	$t-t_0$	$t-t_0/t_0$	η	$(\eta/\eta_0)^{1/3}$	Drug conc. (μM)	DNA conc. (μM)	r	$(\eta/\eta_0)^{1/3}$
20	20.2	0.2	0.01	0.01	26.73	26	0.73	0.0281	0.028	1.2	0	30.0	0	1.2
					26.75		0.75	0.0288	0.029	1.21	2.1		0.07	1.21
					26.8		0.8	0.0308	0.031	1.22	4.2		0.14	1.22
					26.82		0.82	0.0315	0.032	1.21	6.3		0.21	1.21
					26.85		0.85	0.0327	0.033	1.23	8.4		0.28	1.23
					26.89		0.89	0.0342	0.034	1.22	10.5		0.35	1.22

^a Mean of three different determinations.

Table S3: Raw data for Fluorescence emission spectra of the EB-ctDNA complex in presence and absence of DCN at 298 K. C(ctDNA): 30.0 μ M; C(EB): 1.2×10^{-3} M; C(DCN): 0, 2.1, 4.2, 6.3, 8.4, 10.5 μ M

DCN Concentration (μ M)	Fluorescence intensity ^a ($\lambda_{\text{ex}}/\lambda_{\text{em}} = 525/624$ nm)
0	430
2.1	428
4.2	425
6.3	425
8.4	424
10.5	424

^a Mean of three different determinations.

Table S4: Raw data for fluorescence emission spectra of the RB-ctDNA complex in presence and absence of DCN at 298 K. C (ctDNA): 30.0 μ M; C(RB): 2.0×10^{-3} M; C(DCN): 0, 2.1, 4.2, 6.3, 8.4, 10.5 μ M

DCN Concentration (μ M)	Fluorescence intensity ^a ($\lambda_{\text{ex}}/\lambda_{\text{em}} = 465/577$ nm)
0	680
2.1	610
4.2	580
6.3	550
8.4	510
10.5	490

^a Mean of three different determinations.

Table S5: Raw data for the effect of the ionic strength of NaCl on the absorbance of ctDNA-DCN complex. Concentrations of DCN and ctDNA were 6.3×10^{-6} M and 3.0×10^{-5} M, respectively. The concentrations of NaCl: 0, 0.01, 0.02, 0.03, 0.04, 0.05, 0.06, 0.07 M.

NaCl Concentration (M)	Absorbance ^a (at 260 nm)
0	0.323
0.01	0.312
0.02	0.32
0.03	0.316
0.04	0.311
0.05	0.329
0.06	0.319
0.07	0.325

^a Mean of three different determinations.

Table S6: Raw data the plot of $A_0/(A-A_0)$ versus $1/C_{\text{DCN}}$ at different temperature settings ($C_{\text{DNA}} = 3.0 \times 10^{-5} \text{ M}$)

298 K (25 °C)					
A_0^a	A^a	$(A-A_0)$	$A_0/(A-A_0)$	DCN Conc. (μM)	1/ DCN Conc. (L/mol)
0.201	0.258	0.057	4.3125	2.1	476190.476
	0.314	0.113	2.04950	4.2	238095.238
	0.378	0.177	1.26219	6.3	158730.159
	0.453	0.252	0.8625	8.4	119047.619
	0.493	0.292	0.7289	10.5	95238.0952
303 K (30 °C)					
A_0^a	A^a	$(A-A_0)$	$A_0/(A-A_0)$	DCN Conc. (μM)	1/ DCN Conc. (L/mol)
0.207	0.255	0.048	3.5263	2.1	476190.476
	0.308	0.101	1.7787	4.2	238095.238
	0.371	0.164	1.1356	6.3	158730.159
	0.447	0.24	0.7976	8.4	119047.619
	0.491	0.284	0.6884	10.5	95238.0952
313 K (40 °C)					
A_0^a	A^a	$(A-A_0)$	$A_0/(A-A_0)$	DCN Conc. (μM)	1/ DCN Conc. (L/mol)
0.075	0.143	0.068	2.4124	2.1	476190.476
	0.18	0.021	1.3215	4.2	238095.238
	0.215	0.014	0.95763	6.3	158730.159
	0.233	0.032	0.75678	8.4	119047.619
	0.25	0.049	0.6323	10.5	95238.0952

^a Mean of three different determinations.

Table S7: Raw data for the Van't Hoff plot for the ctDNA-DCN complex

1/T (K⁻¹)	K_b (M⁻¹)	lnK_b
0.00336	7.7×10^5	13.6
0.0033	5.5×10^5	13.3
0.00319	3.6×10^5	12.79