

Molecular recognition of parallel quadruplex d-(TTGGGGT)₄ by mitoxantrone: binding with 1:4 stoichiometry leads to telomerase inhibition

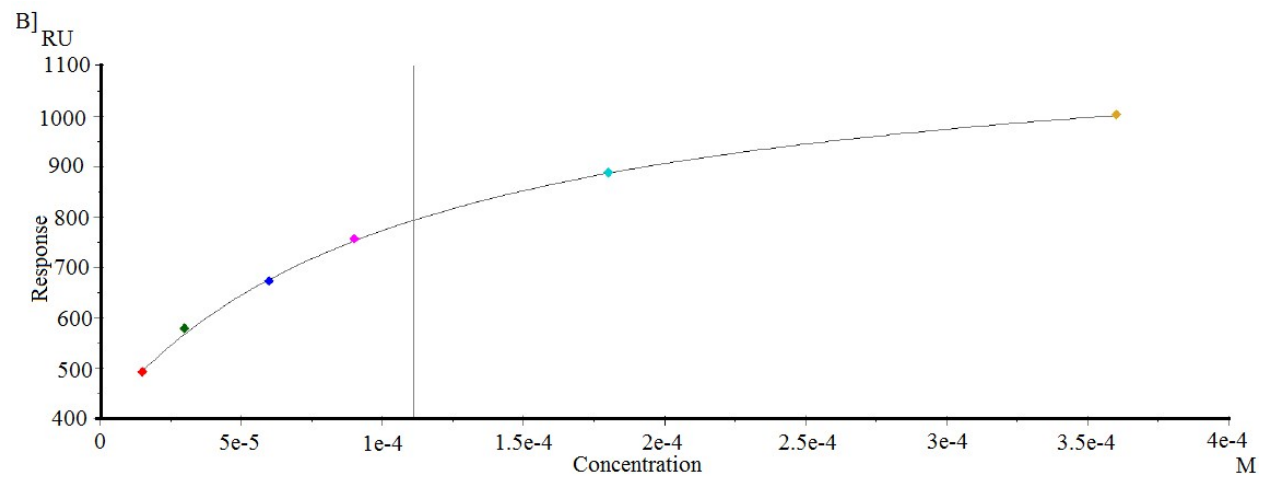
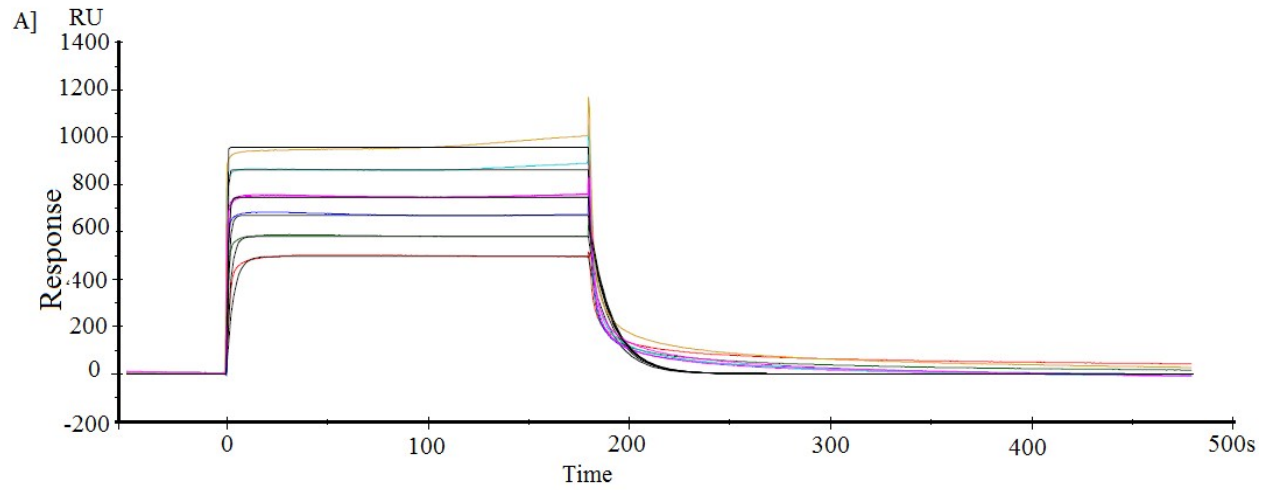
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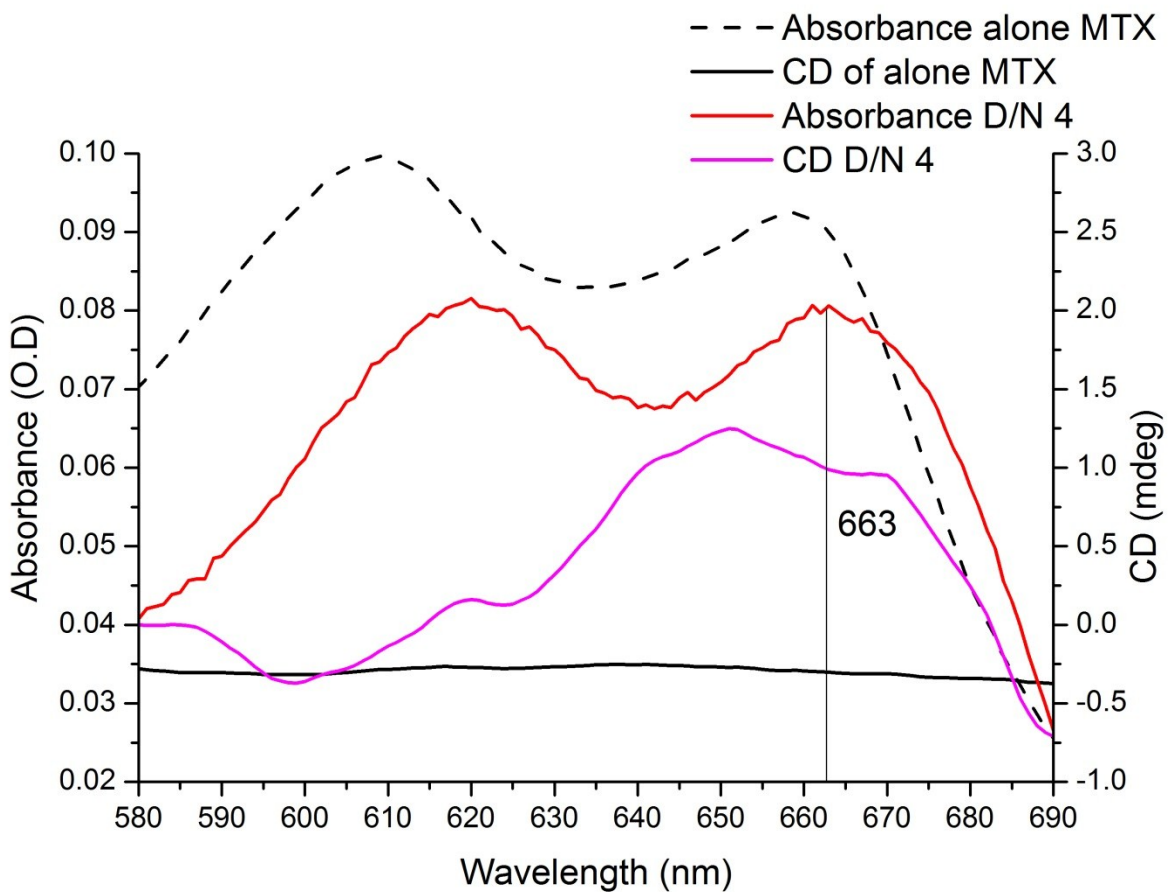
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Supplementary Information

S1: Results of Surface Plasmon Resonance for binding of mitoxantrone to 22-mer d-[5'-GGGG(TTGGGG)₃-3'] using HEPES buffer with 100 mM KCl (A) Sensograms obtained for unbound mitoxantrone concentration of 15, 30, 60, 90, 180 and 360 μ M, from bottom to top curves. (B) Binding plots showing Response Unit (RU) versus concentration of mitoxantrone from steady state data.



S2: Absorbance and CD overlay of uncomplexed MTX and 4:1 d-(TTGGGGT)₄ complexed MTX in 20 mM phosphate buffer with 100 mM KCl at 298 K showing bisignate induced CD band.



SI Table 1: SPR data with equilibrium binding constants for binding of MTX with 7-mer d-(TTGGGGT)₄ and 22-mer d-[5'-G₄(T₂G₄)₃-3'].

Experiment	Flow rate ($\mu\text{l}/\text{min}$)	RU_{max} (RU)	k_a ($\text{M}^{-1} \text{s}^{-1}$)	k_d (s^{-1})	K_D (M)	K_A (M^{-1})	Chi² (RU²)
7-mer (kinetics run 1)	30	1375	1.185×10^4	0.3947	3.33×10^{-5}	3.00×10^4	171.0
7-mer (kinetics run 2)	30	1174	1.134×10^4	0.3236	2.85×10^{-5}	3.50×10^4	354.0
7-mer (steady state run 1)	30	1375	-	-	9.65×10^{-5}	1.03×10^4	358.3
7-mer (steady state run 2)	30	1174	-	-	8.75×10^{-5}	1.14×10^4	308.8
22-mer (kinetics run)	30	663	1.428×10^4	0.0872	6.104×10^{-6}	1.64×10^5	955.0
22-mer (steady state run)	30	460			1.11×10^{-4}	0.91×10^4	402.3