The Supplementary Information for

“Understanding Enhanced Mechanical Stability of DNA in the Presence of Intercalated Anticancer Drug: Implications for DNA Associated Processes”

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FIG. S1. Effect of an intercalator on DNA's inter base pair rise and twist. Rise (a) and twist (b) as a function of the base pairs step (number) are plotted for the bare B-DNA and the two intercalated drug-DNA complexes. The error bar for each step of base pairs in each plot is the standard deviation of 2500 data points obtained from the last 50 ns of simulation time. For each drug intercalated complex, rise for the step of the 6–7 base pairs is ~ 3.5 Å more than that of the bare B-DNA, as an intercalator is present between these two base pairs. Otherwise, the rise is the same both in the presence and absence of an intercalator. Twist for the step of the 6–7 base pairs of the DNA–daunomycin ($= 29^\circ$) and DNA–ethidium ($= 7^\circ$) complexes are much less than that of the B-DNA ($= 36^\circ$). Twist of DNA in the presence of an intercalated drug differs from that of the bare B-DNA maximum up to 3 base pairs on either side of the intercalation site. This represents local unwinding of the DNA double helix structure in the presence of an intercalator, which is more significant for ethidium than daunomycin.

FIG. S2. Comparison of structure and elastic properties of the middle 6 base-pairs of DNA (marked within the rectangle) for the bare B-DNA (a), the DNA–daunomycin (b), and the DNA–ethidium (c) from equilibrium simulations. The representations and colors are the same as shown in Fig. 1 in the main text. Stretch modulus, γ , and persistence length, l_p , (as well as bending rigidity κ) for each system given in Table II in the main text are calculated from the normalized probability distributions of DNA contour length (d) and bending angle (e), respectively. See the calculation details in the main text. The distributions for each system are obtained from the last 50 ns of 200 ns long simulation.

FIG. S3. (i–x) The instantaneous snapshots for shearing of the DNA–ethidium complex by the OS3 pulling protocol are shown at various DNA-extensions as pointed in the force–extension plot in Fig. 8(a) in the main text. The representation and color coding in each snapshot are the same as described in Fig. 1 in the main text.

FIG. S4. (i–viii) The instantaneous snapshots for tearing of the DNA–ethidium complex by the MU protocol are shown at various DNA-extensions as pointed in the force–extension plot in Fig. 8(b) in the main text. The representation and color coding in each snapshot are the same as described in Fig. 1 in the main text.