Supporting Information

A New Bisintercalating Anthracycline with Picomolar DNA Binding Affinity

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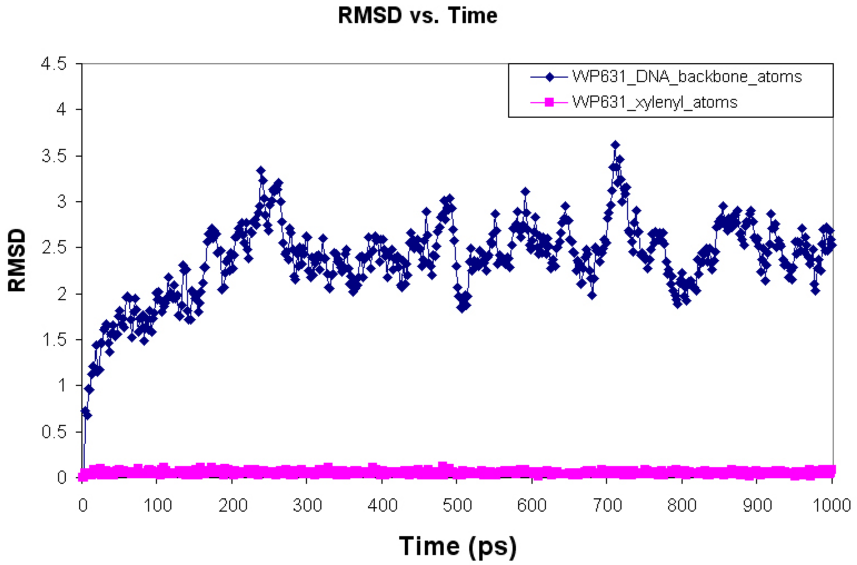
Figure S1. RMSD vs. time (ps) over the molecular dynamics trajectory of WP631 (A) and WP762 (B). The blue line shows the RMSD for the DNA backbone atoms and the red line shows the RMSD for the atoms of the xylenyl linker only.

A.



B.

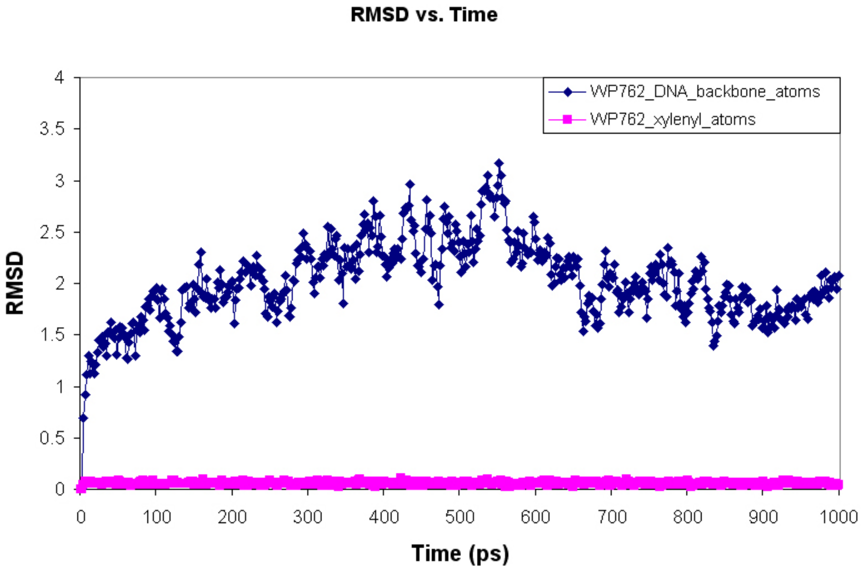
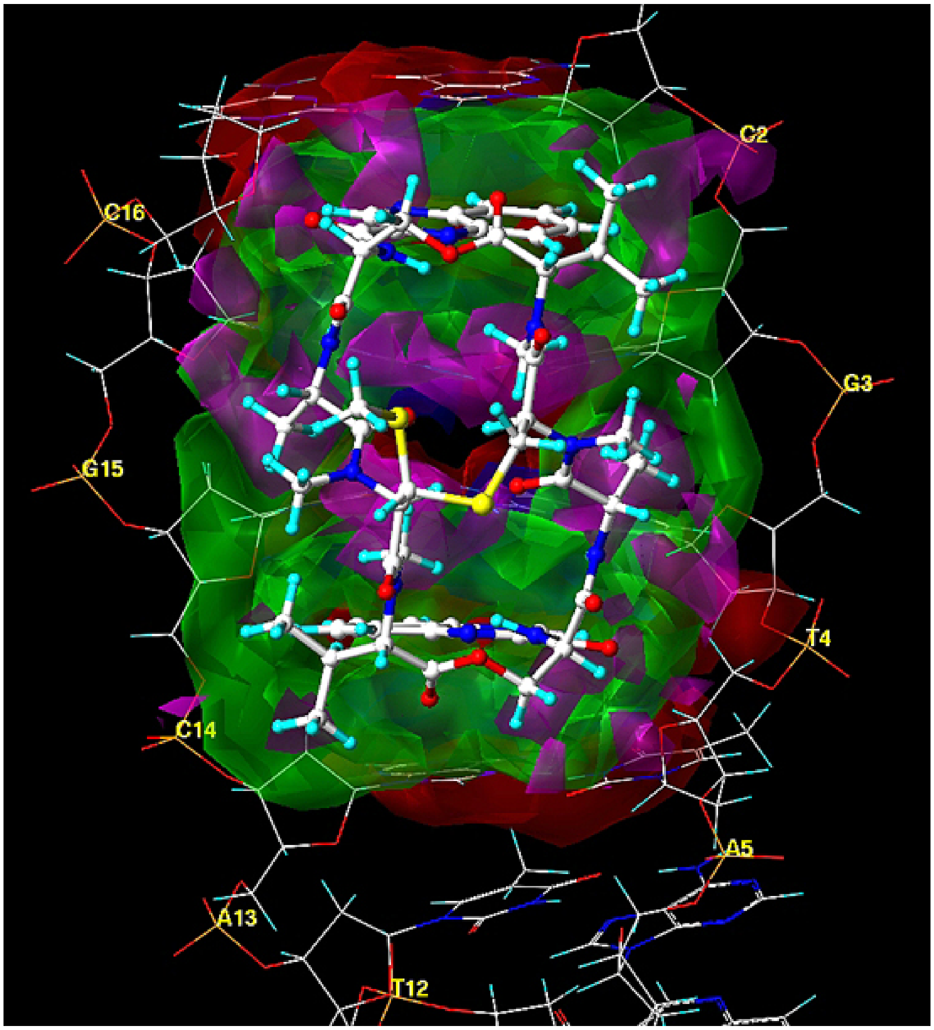


Figure S2. HINT interaction map for the interaction of echinomycin with the 5’-G|CG|T-3’ base pair sequence of DNA, which displays, visually, the quality and magnitude of the various binding contacts involved in the interaction. The contour surfaces are color-coded by interaction type at a constant map density value of ±150. See the description for Figure 6 for the HINT map contour color code descriptions.



Elemental Analysis was calculated for $C_{62}H_{66}Cl_2N_2O_{20}$ x $3H_2O$: C; 57.99, H; 5.65, Cl; 5.52, N; 2.18. Found: C; 58.09, H; 5.64, Cl; 5.62, N; 2.16.