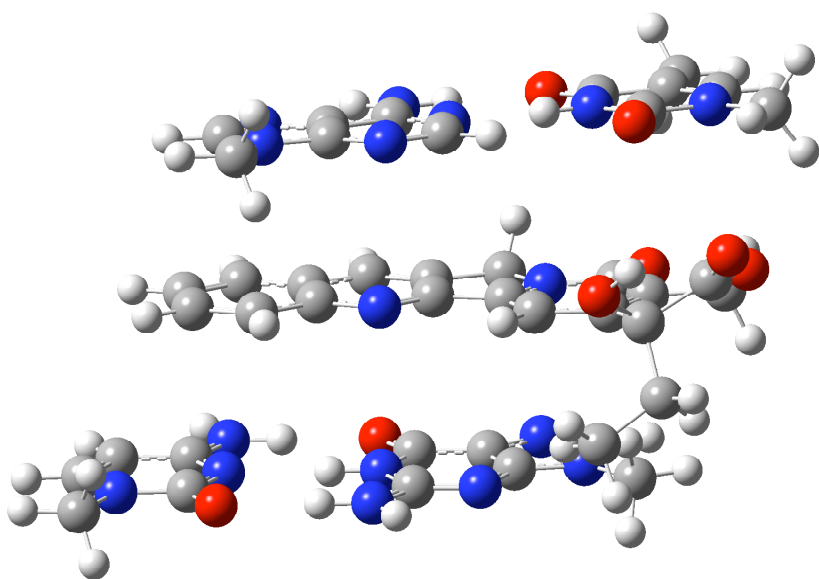


Supporting Information

An Ab Initio Quantum Mechanics Calculation that Correlates with Ligand Orientation and DNA Cleavage Site Selectivity in Camptothecin-DNA-Topoisomerase I Ternary Cleavage Complexes

Xiangshu Xiao and Mark Cushman*

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A

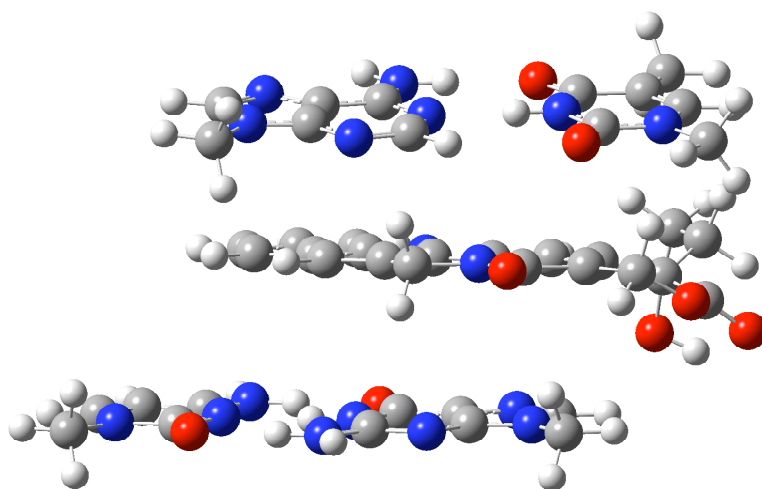
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6	4.953399	1.664906	-.300553
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6	3.898446	1.801488	-2.514780
8	2.922068	2.130796	-3.168018
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6	5.135924	.963547	-4.578700
6	6.087977	.886513	-2.260954
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6	-.635770	4.134394	.062384
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1	3.128780	2.395535	-.730792
1	4.315482	.300901	-4.891590
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B

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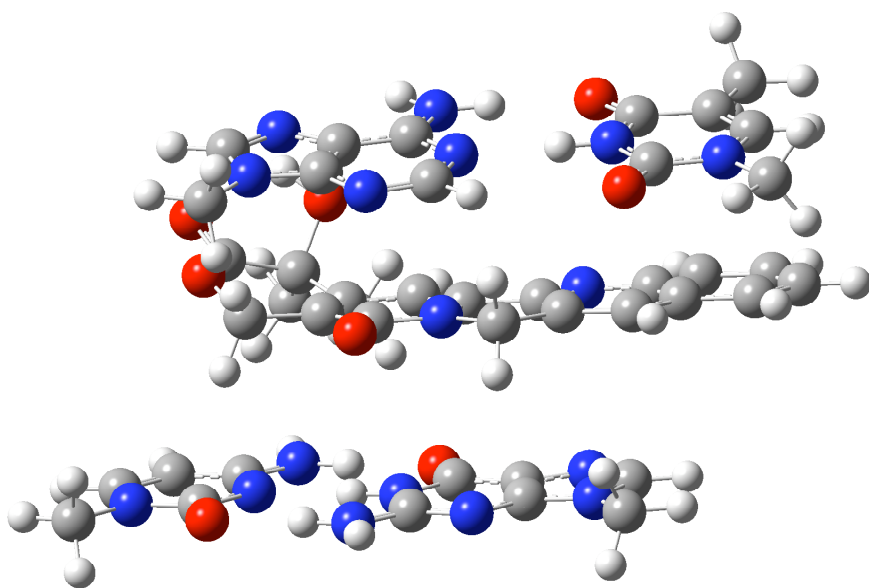
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Atomic number	X	Y	Z
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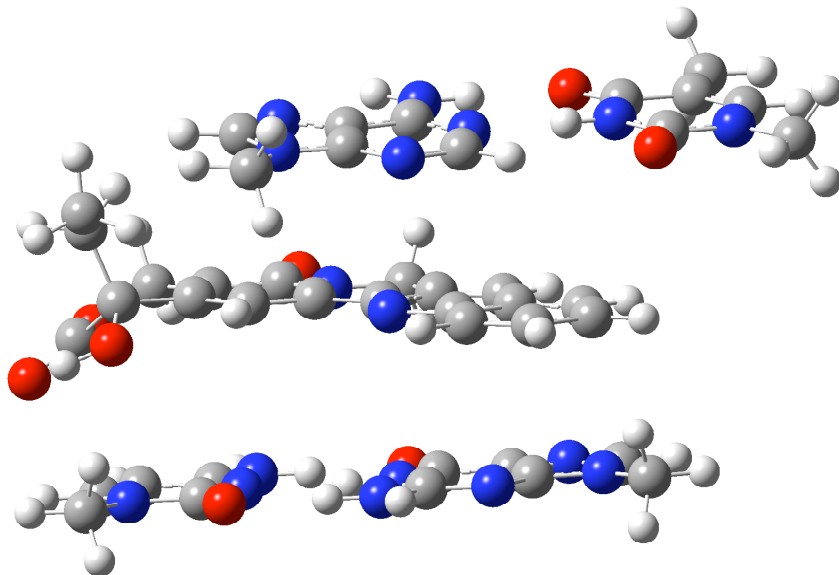
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D

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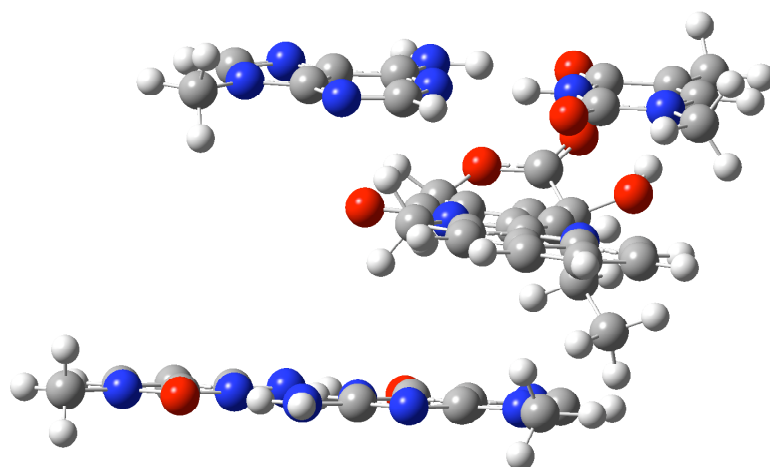
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6	-1.875723	-3.016157	.577121
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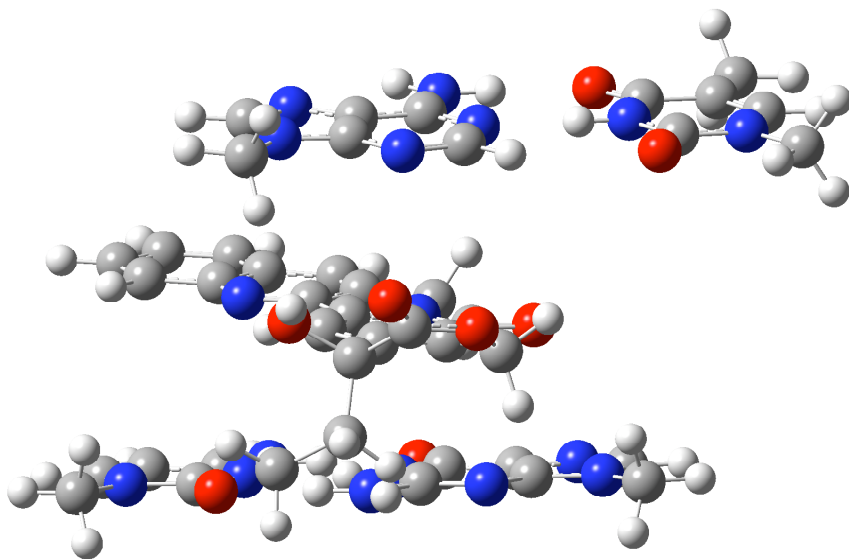
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6	5.661052	.669233	.841780
6	6.111908	2.099024	.915704
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6	-2.463159	-4.368421	4.606440
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6	-.353539	3.470202	.833852
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F

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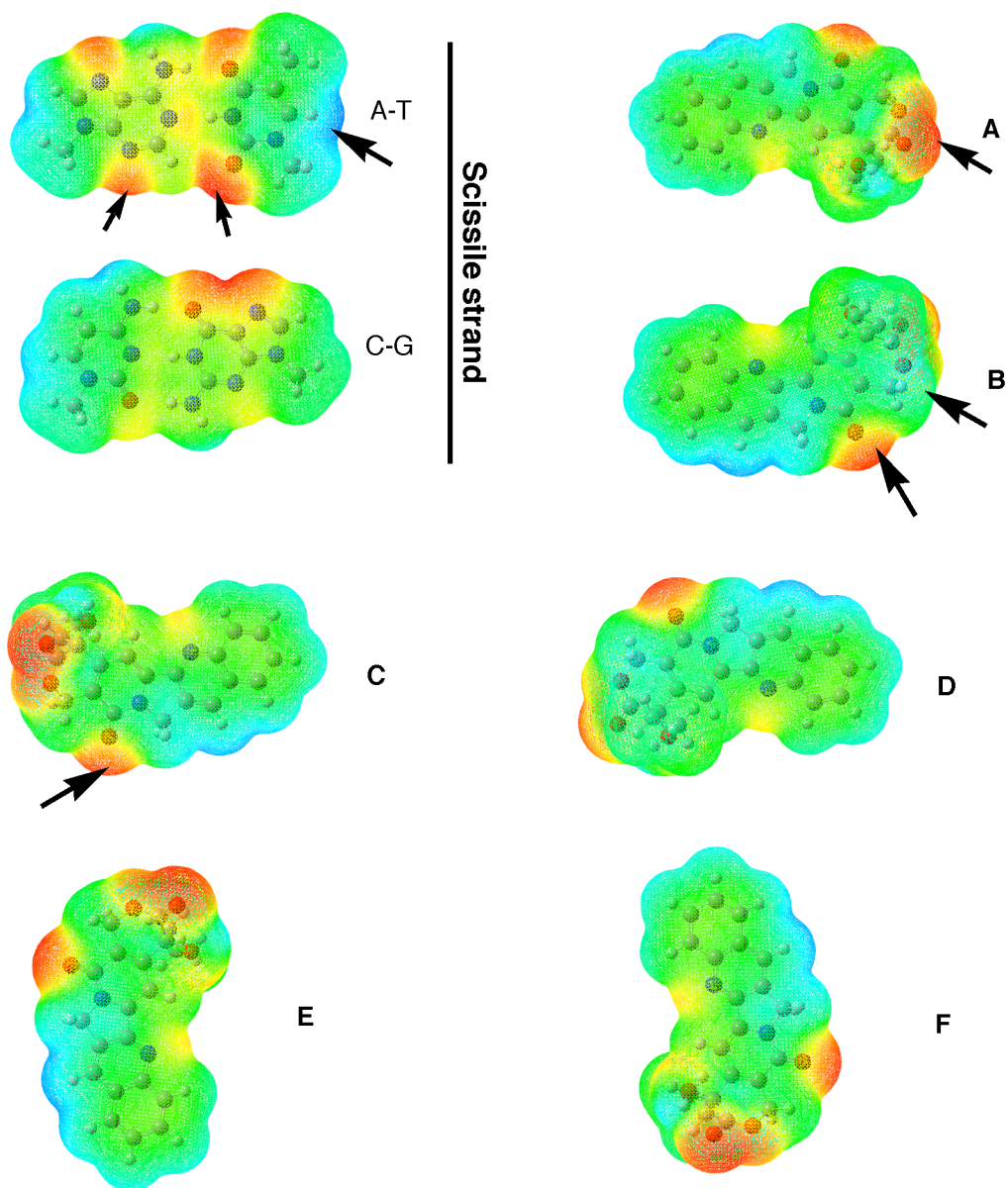


Figure 1S. The electrostatic potential surface maps of A-T, C-G base pairs and CPT mapped on the total electron density calculated at the HF/6-31G** level of theory. The disposition of A-T, C-G and the individual orientations of CPT (**A-F**) are displayed in a way that is similar to the cleavage site models **A-F**. Thus, the scissile side is to the right of A-T and C-G. Red color denotes the electrostatically negative charge and the blue color represents the electrostatically positive charge. The major groove is above and the

minor groove is below each structure. The arrows indicate electrostatic attraction (in **A**) or repulsion (in **B** and **C**) between CPT and base pairs.

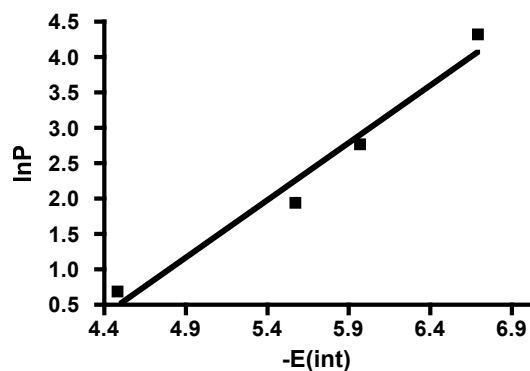


Figure 2S. Correlation between interaction energy (E_{int}) and frequency of CPT-stabilized sites ($\ln P$) in the SV40 genome. The points plotted correspond to the first four entries in Table 2.

Complete list of authors for reference 10:

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